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Canonical correlations in quantum systems

Brecht Dierckx

Dissertation presented in partial fulfilment of the requirements for the degree of Doctor of Science

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□ *(wat gezegd moest worden)*,
Brecht Dierckx

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Contents

CHAPTER 1

Some random thoughts on quantum systems

> Example is the school of mankind, and
> they will learn at no other.
>
> *Letters on a Regicide Peace*
> Edmund Burke

The quantum information community is a melting pot of experimental and theoretical physicists, computer scientists, engineers, mathematicians, and even the occasional philosopher and/or crackpot. This wide spectrum of schooling is reflected in the diversity of results being pursued and published. In broad terms, these can be classified into four major schools of research;

(i) **Quantum communication theory** [1] studies the use of quantum logic to store, transmit, and retrieve either classical or quantum information. Also, researchers in this field are trying to define exactly what the difference is between classical and quantum information.

(ii) **Quantum cryptography** [1] studies the use of intrinsic quantum properties of physical communication channels for cryptographic tasks. Although a myriad of different protocols exist, the key idea behind quantum cryptography is that it is impossible to eavesdrop on quantum communication without being detected by the sender or the intended receiver.

(iii) **Quantum computation theory** [1] aims to leverage the probabilistic quantum logic into a universal computation theory. Its ultimate goal is to build large-scale functional quantum computers which can tackle problems out of reach for classical computers, such as efficient simulation of protein folding.

For some problems, quantum computation theory promises an exponential speedup over classical computation devices.

(iv) **Foundations of quantum mechanics** [2, 3, 4, 5]. Researchers in this field aim to amend our incomplete understanding of quantum theory by providing an information-theoretical framework to replace the standard axioms of quantum mechanics. Among other things, these scientists seek to provide a satisfying answer to the so-called *measurement problem.*

As a group though, the quantum information community aims to push the boundaries of the idea that *information is physical* to the very limits of our theoretical and experimental understanding of the universe(s).

The introduction of information as a physical quantity, and information theory in general, into the framework of quantum mechanics results in some rather strange and perhaps unexpected considerations. Even some of the greatest scientific minds of the modern world have struggled with the implications of this marriage between information theory and quantum mechanics. The probabilistic nature of quantum theory led Albert Einstein to initially reject quantum mechanics as a complete physical theory, stating "*Quantum mechanics is certainly imposing. But an inner voice tells me that it is not yet the real thing. The theory says a lot, but does not really bring us any closer to the secret of the 'old one'. I, at any rate, am convinced that He [God] does not throw dice.*". Eistein also derided the notion of entanglement, which plays a pivotal role in quantum information theory, as 'spooky action at a distance', since in his mind, it violated the idea that information cannot be transmitted faster than at the speed of light.

Even though few physicists today share Einstein's specific objections to quantum mechanics, the theory is still littered with enough strange concepts and ideas to divide physicists on the question of how the mathematics of quantum mechanics should be interpreted as a physical theory. Currently, there are over a dozen possible interpretations to bridge this gap between mathematics and reality.

This division over how quantum mechanics should be interpreted, can, to a large degree, be reduced to our inability to integrate our macroscopic understanding of the universe in a quantum mechanical setting. We can create the machinery to probe the very building blocks of the universe, but we only have a heuristic understanding of *how* such a machine is able to give us any measurement results. We can measure the spins of individual electrons, but fail to understand the process that produces the up-or-down result on our computer screens. We turn some knobs and tighten some screw and somehow, almost magically, a $\uparrow$, a $+$, a 1 appears on our computer screen to tell us that by turning that knob and tightening that screw, we have 'measured' the spin of an electron and it's $\uparrow$ or $+$ or 1.

If quantum mechanics is really the language of the universe, then turning a knob or tightening a screw should also be described by quantum mechanics, just like the single electron that we are studying. If we look at that screw under a microscope, then we see that it is indeed composed of electrons, neutrons and protons, all particles that move according to the rules of quantum mechanics. Yet

no physicist in his right mind would ever attempt to describe all those electrons, protons, and neutrons in that screw as a single quantum system.

The problem with such an attempt is one of scale. There are simply too many electrons, protons and neutrons to keep track of and each additional electron or proton doubles the effort it takes to describe such a system using the quantum formalism. Not even the fastest computers in the world can keep up with such systems. In fact, the best we can do at the moment, is simulating about 15 electrons simultaneously and if Moore's law keeps up, then in two years time, we will be able to simulate 16. In another two years, 17 and it would take roughly till the end of the universe before we can simulate just one single little screw.

The realization that attempting to describe macroscopic objects by keeping track of the individual microscopic constituents and applying the laws of quantum mechanics to those objects is futile, has led physicists to consider statistical techniques that interpolate between this microscopic quantum world and the macroscopic classical world in which we live.

In this thesis we discuss two rather distinct statistical approaches for describing large scale quantum systems. In reverse chronological order, these are approaches based on free random variables and quasi-free fermionic structures. In spite of what their names might suggest, both are rather different approaches to deal with complexity in quantum systems. This distinction is reflected in the structure of this document. Chapter 2 deals with quasi-free structures in quantum information theory, and chapter 3 and 4 deals with the constructing of a reduced description using free random variables. Both parts are self-contained with their own proper introduction and conclusions. The current chapter does contain two short primers on these subjects, before we paint a more complete picture in the following chapters.

The quasi-free approximation

Most descriptions of large quantum mechanical systems rely on either approximations or specialize to specific types of systems which reduce the complexity of characterizing the states of a quantum system. One very successful such scheme is the quasi-free approximation. For systems of bosons or fermions, only states with a particular combinatorial structure are considered. Very roughly speaking, such quasi-free states are the bosonic and fermionic analogues of independent particles in a quantum setting. Any multi-particle quasi-free state is completely determined by the two-point correlation functions associated to that state. That is, if we know how any two particles behave, than we can calculate efficiently how any three or more particles behave.

By restricting ourselves to the study of quasi-free states, we effectively reduce the complexity of calculating physical quantities exponentially. For bosonic systems, this feature was recognized early on by the quantum information theory community and a wealth of results on such systems have been published. In contrast, the fermionic quasi-free systems have gone largely unnoticed by the same community.

In chapter 2, we wil look at quasi-free fermionic systems from an information-theoretical point of view and how the quasi-free approximation can be of use to the quantum information theory community. To that end, we deduce reduced expressions for several entropic measures. Additionally, we completely characterize the set of dynamical evolutions which are amenable to the quasi-free structure of our states.

Household interactions in quantum mechanics

One of the crown achievements of quantum mechanics is the description of all possible dynamical evolutions a finite quantum system can undergo in terms of Kraus operators. In the Schrödinger picture, this means that for any time t, the time evolution of a density matrix ρ describing a physical system at time $t = 0$ can be expressed as

$$\alpha_t(\rho) = \sum_k V_k \rho V_k^*, \tag{1.1}$$

such the Kraus operators V_k satisfy a normalization condition,

$$V_k^* V_k = \mathbb{1}. \tag{1.2}$$

Although there is still some debate [6] on whether this classification is complete, it is hard to argue against the defining characteristics of evolutions described by (1.1). Any such evolution of a system is linear and amenable to imbedding the system in a larger system, i.e. completely positive. Such an imbedding not only allows for a joint description of multiple systems, it can also be shown that any evolution described by Kraus operators can be written as a truncation of a unitary time evolution of a larger system, i.e. there exists a density matrix σ and Hamiltonian H such that

$$\alpha_t(\rho) = \mathrm{Tr}_2\, e^{itH} \rho \otimes \sigma e^{-itH}. \tag{1.3}$$

Evolutions described by Kraus operators are thus exactly those which have a nice system-environment representation.

At the same time, evolutions of the form (1.1) are the only evolutions which have the above characteristics and so one could argue that linearity and complete positivity serve as a minimal set of physical requirements for a realistic evolution of a quantum system.

This presupposed equivalence between physical evolutions and their mathematical representation in terms of Kraus operators has had a massive impact on quantum information theory. For information-theoretical questions, the traditional picture of small, controllable systems in contact with a large, inaccessible environment has largely been abandoned in favor of a black box description[1] in terms of Kraus operators.

[1] In classical discrete information theory, a similar shift occurred in the twentieth century. The

There are many reasons for this focus on Kraus operators, but perhaps the most pertinent one is the computational ease. The physically relevant environment of a system under observation is often quite large, much larger than the system itself. Explicitly computing a time evolution as in (1.3) is not an easy problem. For finite systems, the Hamiltonian H is a finite-size matrix and the most computationally intensive task is diagonalizing this matrix H. For generic Hamiltonians, the computational complexity of this task scales with the cube of the size of the matrix.

The corresponding description in terms of Kraus operators only involves multiplications of matrices of a size corresponding to the size of the system under observation. The system size is often negligible compared to the size of the environment and so computing the evolution becomes a much more manageable problem.

Although mathematically equivalent, determining a set of Kraus operators for a system-environment interaction is often impractical if not impossible. It is easier to go the other way around and derive a system-environment representation for a system undergoing an evolution as in (1.1). However, such a representation is not unique and by no means should such a representation be interpreted as the underlying 'actual' physical process. Any completely positive evolution of a finite system can be represented as a system-environment interaction on a space only twice the size of the original space. For a qubit whose underlying Hilbert space is $\mathbb{C}^2$, any completely positive map acting on this qubit can be represented as a truncation of a unitary evolution on $\mathbb{C}^4$. Typically, the relevant environment of any physically implemented qubit will be far larger than this and so a representation on $\mathbb{C}^4$ will not correspond to the actual physical process summarized by an interaction of the form (1.1).

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focus of research came to rest on the logical operations permitted on a string of bits, rather than on the physical interactions implementing them. The benefits of this were huge, as this allowed scientists to study information and computation models independently from the physical systems which actually implemented them. Perhaps the most physically striking result which came about as a consequence of this program was Shannon's noisy coding theorem, which effectively set bounds for the amount of information which can be exchanged between classical physical systems. It also confirmed the intuitive idea that two identical information transmission channels should be able to transmit information twice as as fast as one of these channels.

It should thus not come as a surprise that a similar program was attempted in quantum information theory and for many years, decades even, the hunt was on for a quantum analogue of Shannon's noisy coding theorem. This hunt came to a, for many, abrupt end when it was shown by Hastings and others that, in contrast to the classical case, quantum systems can have wildly different behavior when it comes to their information transmission capacities. For some, the old classical rule that two identical systems are exactly twice as good at transmitting information as one of these systems still holds. For the new examples by Hastings, it fails dramatically and somehow quantum mechanics allows for superadditive behavior. Unfortunately, there is, as of yet, no clear answer to the question why it should fail.

One of the major hurdles in tackling this problem is exactly this dichotomy between the logical operation description (Kraus operators) and the physical processes implementing them. So, although we know that systems should exist which violate Shannon's theorem on a quantum level, we have no idea what these systems, or more to the point, their environments are; what type of particles make up these environments, if there is a temperature dependence, if a temperature can be defined at all.

Unfortunately, this means there is a rather large gap between the two descriptions and the mathematical convenience of Kraus operators has to be weighed against the use of physically motivated parameters such as the temperature or pressure of the environment in dynamical models.

Intermediate level description in terms of master equations can bring some relief to this matter. The temperature of the environment is often a conveniently accessible parameter in such a description. The tradeoff for this is imbedded in the derivation of such master equations. With a few exceptions, master equations describing dissipative evolutions of quantum systems rely on a weak coupling limit or other types of approximation. While the coarse-grained behavior of quantum systems can often be described rather well by such approximations, the short timescales required for quantum computation drive us to consider less restrictive schemes.

In chapter 4 we consider a composite system consisting of a tightly controllable quantum system in contact with a large, mostly inaccessible environment. The interaction between the system of interest and the environment is assumed to be composed of large unitarily invariant random matrices. Such models have been considered before in [7, 8, 9, 10, 11, 12, 13].

It is our aim to trace out the interaction terms and in doing so obtain reduced states and dynamics of the stable observables. This problem is generally intractable unless we limit our attention to an extreme form of randomness for the coupling observables, namely to the asymptotic regime of suitably scaled high dimensional random matrices.

In this limit, the randomness of the interaction terms freezes and mixed moments of both the interaction terms and the unperturbed Hamiltonian become deterministic; the unperturbed Hamiltonian and the interaction terms converge asymptotically to a free family of random variables. Alternatively, if sufficient structure is imposed on the nature of the interaction terms, the family can be free with amalgamation over the algebra of system observables.

The emergence of freeness in this model effectively reduces the information needed to describe the time evolution of the system of interest to an understanding of the spectral properties of the interaction terms and of the full operator structure of the unperturbed Hamiltonian. If we additionally assume that the initial state of the environment is invariant under the unperturbed dynamics, the needed information further reduces to only knowledge of macroscopic properties of the initial environmental state and spectral properties of the unperturbed Hamiltonian and the interaction terms. It then becomes feasible to explicitly calculate the dynamical behavior of observables associated to the system of interest, irrespective of the type of environment.

It should be stressed that no approximations like replacing Hamiltonians by effective Hamiltonians, assuming particular decoupling schemes or assuming the existence of well-separated time scales are involved. Not surprisingly, the equations governing such reduced dynamics are quite complicated, but some simple cases can be analyzed.

Outline of the thesis

This documents consists of two main parts and three chapter. To elucidate the underlying structure of this thesis, we provide a brief outline.

- Chapter 2 is self-contained. The basic concepts of fermionic systems and quasi-free structures in quantum mechanics are briefly introduced and references to more complete reference works are provided for the interested reader.

  Next, we introduce the protagonists in our quasi-free story, the exponential elements. The basic properties of this elements are deduced and quickly put to use to prove main results of this chapter.

  As a first application, we derive reduced formulas to calculate various entropic measures for generic quasi-free states. These formulas reduce the complexity of these measures exponentially; they only require knowledge of the one-particle state.

  The second novelty in this chapter is the full classification of all positive linear maps which preserve the quasi-free nature of quantum states. The completely positive maps which preserve the quasi-free nature are also identified and explicit conditions are derived which characterize them in full.

- Chapter 3 is a crash course in free probability, which is the main tool used in chapter 4. The knowledgeable reader is still invited to flip through this chapter as some non-standard nomenclature and notation are introduced in this chapter.

- In chapter 4 we consider composite systems consisting of a tightly controllable quantum system in contact with a large, mostly inaccessible environment. The interaction between the system of interest and the environment is assumed to be composed of large, unitarily invariant random matrices. In the limit of an infinite environment, these unitarily invariant random matrices converge to an (amalgamated) free family of random variables.

  In this limit, the random correlations between the interaction terms and the unperturbed Hamiltonian freeze and an almost deterministic dynamics appears. This dynamics is investigated using the results introduced in chapter 3. Unfortunately, the existing techniques in free probability theory do not suffice to analyze such quantum mechanical systems properly. A large part of this chapter is thus devoted to the development of new techniques which do allow an in-depth study of these systems.

  Using these new techniques we then study the dynamics of such freely interacting systems and derive general equations which describe such systems. To illustrate the general results, we discuss some explicit examples.

This thesis deals with two rather different notions of canonical correlations in quantum mechanics. The first part coincides with the first chapter and deals

with quasi-free structures in quantum information theory. The second part consists of chapters three and four and deals with free structures in quantum mechanics. Contrary to what their names suggest, quasi-free and free structures are completely different in both their nature and philosophy. As such, there is no 'conclusions' chapter at the end of this thesis. The final section of chapters 2 and 4 subsume the role of a central conclusions chapter and tie up the loose ends for each part.

CHAPTER 2

Quasi-free structures in quantum information theory

There are not too many classes of states or quantum operations that can be handled in detail. Well-known examples of tractable classes are gaussian structures in bosonic systems [14], free structures in non-commutative probability theory[1] and exchangeable states and maps for spin systems [15, 16]. Although the systems under consideration can often be quite large, even infinite, the computational complexity of most associated quantities in these settings is many orders of magnitude lower than what one encounters in more general systems. Gaussian states in particular have been used in quantum optics to that effect for many years.

Perhaps because of the close link between the two fields, gaussian states were also the first of the aforementioned classes to come under consideration in quantum information theory. Recent years have seen a large amount[2] of work done on their role in bosonic systems, see for instance [17].

Rather remarkably, the fermionic counterparts to gaussian structures, quasi-free fermionic systems [14], do not share the same popularity in the quantum information community as their bosonic cousins. In field theory and statistical mechanics, such effective free evolutions and states have been used extensively as an approximation to interacting systems, a well-known example being the Hartree-Fock approximation. Even more so than for bosonic systems the Fermi statistics often dominates the interaction and effective quasi-free approximations tend to be quite realistic, though much more tractable.

The main simplifying feature lies in the particular combinatorial properties of

[1] These will be analyzed in chapters 3 and 4.

[2] Merely typing in the keyword 'gaussian' in the quantum theory frontend of the arxiv returns at present over 250 research papers.

correlation functions of states and dynamical mappings. In fact, the states and dynamics are fully determined by one-particle operators. As the dimension of the observables increases exponentially with the dimension of the one-particle space we obtain a very significant reduction of complexity.

Fermionic systems and quasi-free states should be of particular interest to information theorists. Any N-qubit system can be mapped on an interacting system of fermions by the so-called Jordan-Wigner isomorphism. A particular subset of quantum operations on qubits can then be identified with quasi-free evolutions of fermionic systems and in these problems quasi-free states play an important role. A recent article dealing with this duality between fermions and qubits is [18].

The connection between interacting fermions and general qubit system is not a mere mathematical curiosity. Many of the proposed physical realizations of quantum computers are implementations in systems of fermions. However the actual encoding of qubits is done in such systems, the underlying physical reality determines the stability and usefulness of a quantum computer.

In this chapter we summarize some known results on quasi-free states and introduce a convenient computational tool, dubbed *exponential elements*. These exponential elements allow us to efficiently compute reduced formula's for entropic quantities which are of interest to the quantum information community.

In addition to this, we derive a full characterization of all completely positive and positive maps which preserve the quasi-free nature of states. Before, only a subset of these maps were known.

A word on notation

The symbol $\otimes$ is well-known as a notation for the tensor product of two or more objects. In this chapter, we will use the symbol $\wedge$ to denote the antisymmetric tensor product of vectors, operators and even algebras. Although the meaning of the symbol will change depending on the setting in which it is used, restricting ourselves to a single symbol greatly simplifies the notation and looks, at least to a physicist's eye, more elegant. As is often the case with degenerate notations, the context should specify which version of the wedge we are talking about.

2.1 Algebraics of fermionic systems

The quantum mechanical description of many-particle systems, and in particular systems of fermions, is firmly connected to the mathematical concept of Fock spaces. Given a d-dimensional Hilbert space $\mathcal{H}$ which describes the possible pure states of a single particle, a system consisting of arbitrarily many such particles can be linked to a particular[3] infinite-dimensional separable Hilbert space $\Gamma(\mathcal{H})$, called

[3]It is an interesting observation of Hilbert space theory that any finite dimensional Hilbert space $\mathcal{H}$ results in the same $\Gamma(\mathcal{H})$. More precisely, for any two finite Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, $\Gamma(\mathcal{H}_1)$ is isomorphic to $\Gamma(\mathcal{H}_2)$. Physically this could be summarized as: "Full Fock space doesn't

full Fock space,

$$\Gamma(\mathcal{H}) = \bigoplus_{k=0}^{\infty} \otimes^k \mathcal{H}. \tag{2.1}$$

Every vector in this space corresponds to a possible pure state of a system with an unspecified number of particles. The k^{th} summand in (2.1),

$$\otimes^k \mathcal{H} = \underbrace{\mathcal{H} \otimes \ldots \otimes \mathcal{H}}_{k \text{ factors}} \tag{2.2}$$

describes a system with exactly k particles. Any vector which belongs to this Hilbert space $\otimes^k \mathcal{H}$ is called a k-particle vector and the associated state a k-particle pure state.

The nature of fermions, which have to obey the Pauli exclusion principle, restricts the possible multi-particle states to those which are antisymmetric under permutation of the Hilbert space factors in (2.2). The pure k-particle states are thus all of the form,[4]

$$\varphi_1 \wedge \varphi_2 \wedge \ldots \wedge \varphi_k := \frac{1}{\sqrt{k!}} \sum_{\sigma} \epsilon(\sigma)\, \varphi_{\sigma(1)} \otimes \varphi_{\sigma(2)} \otimes \ldots \otimes \varphi_{\sigma(k)}\,,$$

where σ runs over all permutations of the k indices and $\epsilon(\sigma) = \pm$ depending on the parity of the permutation, $+$ if even, $-$ if odd. The Hilbert space which is spanned by all such linear combinations is denoted $\wedge^k \mathcal{H}$ or $\mathcal{H}^{(k)}$ and the corresponding subspace $\Gamma_a(\mathcal{H})$ is called an antisymmetric or fermionic Fock space,

$$\Gamma_a(\mathcal{H}) := \bigoplus_{k=0}^{\infty} \mathcal{H}^{(k)}.$$

Remark that the dimension of this Hilbert space is only 2^d whereas full Fock space is an infinite-dimensional vector space. This also means that the antisymmetric Fock spaces depend on the number of degrees of freedom of a single particle, in contrast to full Fock space, which is oblivious to the degrees of freedom of a single particle and even to the notion of a particle itself.

Mixed states and observables

An operational description, which allows for open systems containing fermions, requires an algebraic framework which is consistent with the Hilbert space setting we introduced above. Depending on the level of accuracy or the type of processes, which are considered relevant for the problem at hand, different algebraic settings can be used. Below we introduce three such settings where the last two can be considered reduced descriptions of their predecessor: the CAR-algebra, the GICAR-algebra and quasi-free systems, which are not strictly identified with a

count degrees of freedom."

[4] This expression is sometimes called a Slater determinant.

proper algebra, but only with a subset of algebraic operations. Quasi-free system are the central notion in this chapter and so the description of quasi-free structures has been split off into two proper sections, section 2.2 which introduces quasi-free states and section 2.3 which expands on quasi-free maps.

2.1.1 The canonical anticommutation relations

Fermionic Fock spaces can also be constructed in a different way. Any vector φ of a d-dimensional Hilbert space $\mathcal{H}$ induces a linear operator $a^*(\varphi)$ from $\mathcal{H}^{(k)}$ to $\mathcal{H}^{(k+1)}$. The action of $a^*(\varphi)$ is first given on elementary vectors and then linearly extended to the whole space,

$$a^*(\varphi)(\psi_1 \wedge \ldots \wedge \psi_k) := \varphi \wedge \psi_1 \wedge \ldots \wedge \psi_k.$$

The operator $a^*(\varphi)$ is called a creation operator, its adjoint, $a(\varphi)$, an annihilation operator. In effect, they emulate the addition or removal of a single fermion in the state φ to or from a system of fermions . By repeatedly applying creation operators to the vacuum vector Ω, we can build up the entire fermionic Fock space,

$$\psi_1 \wedge \ldots \wedge \psi_k = a^*(\psi_1) \ldots a^*(\psi_k)\,\Omega\,.$$

Although we will not use this language very frequently, the operators defined above satisfy exactly the canonical anticommutation relations required for a quantum mechanical description of fermions,

$$\{a(\varphi), a(\psi)\} = 0 \qquad \text{and} \qquad \{a(\varphi), a^*(\psi)\} = \langle \varphi\,,\, \psi \rangle\, \mathbb{1}. \tag{2.3}$$

The C^*-algebra generated by the creation and annihilation operators is called the CAR algebra in reference to the important commutation relations (2.3). It coincides with the algebra of linear transformations of the antisymmetric Fock space $\Gamma_a(\mathcal{H})$. This algebra is in fact a universal algebra since it is the unique C^*-algebra generated by a unit element $\mathbb{1}$ and by $\{a(\varphi) : \varphi \in \mathcal{H}\}$ such that the operators $a(\varphi)$ satisfy the CAR conditions and that the map $\varphi \mapsto a(\varphi)$ is complex antilinear. We denote it by $\mathfrak{A}(\mathcal{H})$.

The following lemma will be needed later on. It is well-known, so we state it without proof, see [14].

Lemma 2.1. *Suppose that ω is an even state, i.e. vanishes on monomials in creation and annihilation operators with an odd number of factors, on $\mathfrak{A}(\mathcal{H})$ and that σ is a state on $\mathfrak{A}(\mathcal{K})$; then there exists a unique state $\omega \wedge \sigma$ on $\mathfrak{A}(\mathcal{H}) \wedge \mathfrak{A}(\mathcal{K}) := \mathfrak{A}(\mathcal{H} \oplus \mathcal{K})$ defined by*

$$(\omega \wedge \sigma)\,(xy) := \omega(x)\,\sigma(y), \qquad x \in \mathfrak{A}(\mathcal{H}),\, y \in \mathfrak{A}(\mathcal{K}).$$

-

The wedge product $\mathfrak{A}(\mathcal{H}) \wedge \mathfrak{A}(\mathcal{K})$ we implicitly defined in the above lemma is quite different from the tensor product of the two algebras as can be seen from the following constructive explanation.

$\mathfrak{A}(\mathcal{H}_1)$ can be naturally imbedded into $\mathfrak{A}(\mathcal{H}_1 \oplus \mathcal{H}_2)$,

$$\jmath_1 : \mathfrak{A}(\mathcal{H}_1) \hookrightarrow \mathfrak{A}(\mathcal{H}_1 \oplus \mathcal{H}_2) : \jmath_1(a(\varphi_1)) = a(\varphi_1 \oplus 0), \quad \varphi_1 \in \mathcal{H}_1,$$

and of course $\mathfrak{A}(\mathcal{H}_2)$ can be embedded by an analogous mapping $\jmath_2$. Clearly, $\jmath_1(\mathfrak{A}(\mathcal{H}_1))$ and $\jmath_2(\mathfrak{A}(\mathcal{H}_2))$ generate $\mathfrak{A}(\mathcal{H}_1 \oplus \mathcal{H}_2)$, but they do not sit in $\mathfrak{A}(\mathcal{H}_1 \oplus \mathcal{H}_2)$ as tensor factors since,

$$\left\{a^{\#}(\varphi_1 \oplus 0)\,,\, a^{\#}(0 \oplus \varphi_2)\right\} = 0 \quad \text{instead of} \quad \left[a^{\#}(\varphi_1 \oplus 0)\,,\, a^{\#}(0 \oplus \varphi_2)\right] = 0,$$

where $a^{\#}$ denotes either a or a^*. To make the distinction clear, $\mathfrak{A}(\mathcal{H}_1 \oplus \mathcal{H}_2)$ or $\mathfrak{A}(\mathcal{H}_1) \wedge \mathfrak{A}(\mathcal{H}_2)$ is sometimes called the *graded* tensor product of $\mathfrak{A}(\mathcal{H}_1)$ and $\mathfrak{A}(\mathcal{H}_2)$.

Reduced descriptions

Although the CAR algebra is universal, it is not the only possible algebraic description of fermions. Often it is desirable to have a simpler setting which is computationally less complex, but still non-trivial for the problem at hand. We will introduce two such reduced descriptions: gauge invariant and quasi-free systems. The latter is not strictly speaking a complete description of fermionic quantum systems, it is not tied to any well-defined algebra of observables, rather it concerns a particular subset of observables (and states) which all have particular correlation functions. Because of this, a quasi-free descriptions lacks certain features common to algebraic descriptions such as a convex state space. However, quasi-free systems are computationally very convenient, and as stated in the introduction to this chapter, can serve as a reasonable approximation of the more general settings.

2.1.2 The gauge invariant CAR algebra

For any orthonormal one-particle basis $\{e_i\}$ of a d-dimensional Hilbert space $\mathcal{H}$, a special operator can be defined

$$N := \sum_i a^*(e_i)a(e_i). \tag{2.4}$$

This operator is not only invariant under the gauge group $U(1)$ of $\mathfrak{A}(\mathcal{H})$, but also under any unitary basis transformation of the one-particle space and so (2.4) uniquely defines an operator in the algebra independent of the chosen basis.

Consider the action of N on an arbitrary (nonzero) k-particle vector:

$$N\,\varphi_1 \wedge \ldots \wedge \varphi_k = k\,\varphi_1 \wedge \ldots \wedge \varphi_k.$$

N 'counts' the number of particles in a given state and as such is called the *number operator*. Its eigenspaces are the antisymmetric k-particle spaces and its spectrum

consists of the integers $\{0, \ldots, d\}$, which correspond to the number of particles in the associated eigenstate.

The commutant of the number operator is called the gauge invariant CAR or GICAR algebra for short. It is the largest subalgebra of $\mathfrak{A}(\mathcal{H})$ that is invariant under the gauge group $U(1)$. It is also generated as the span of all monomials in a, a^* containing as many a's as a^*'s.

Often the self-adjoint elements in this algebra are identified with the physically accessible observables in a system, since the $U(1)$ group is a gauge symmetry and thus not directly detectable.

Exponential elements

For any d-dimensional one particle space $\mathcal{H}$, the GICAR algebra $\mathfrak{A}^{\mathrm{GICAR}}(\mathcal{H})$ is isomorphic to

$$\mathbb{C} \oplus \mathcal{M}_d \oplus \mathcal{M}_{d(d-1)/2} \oplus \cdots \oplus \mathbb{C}.$$

where $\mathcal{M}_k(\mathbb{C})$ is the k-dimensional complex matrix algebra. The dimension of $\mathfrak{A}^{\mathrm{GICAR}}(\mathcal{H})$, seen as a complex vector space, is $\binom{2d}{d}$.

Remark that the GICAR is an algebra of block diagonal transformations of the antisymmetric Fock space, in particular it contains elements of the form

$$\mathsf{E}(X) := 1 \oplus X \oplus (X \otimes X)\big|_{\mathcal{H}(2)} \oplus \cdots \oplus (\otimes^d X)\big|_{\mathcal{H}(d)}$$

or with an obvious notational meaning

$$\mathsf{E}(X) = 1 \oplus X \oplus (X \wedge X) \oplus \cdots \oplus (\wedge^d X).$$

We will refer to these E-operators as exponential elements[5].

The spectrum $\sigma\Big(\mathsf{E}(X)\Big)$ of an exponential element can be computed to be

$$\sigma\Big(\mathsf{E}(X)\Big) = \left\{ \prod_{i \in \Lambda} \lambda_i \,:\, \lambda_i \in \sigma(X) \,\&\, \Lambda \subset \big\{1, \ldots, \mathrm{Rank}(X)\big\} \right\}.$$

This property is easily verified by looking at the antisymmetric part of $\otimes_k X$. As a tensor product, the eigenvalues of this are exactly all possible monomials of the eigenvalues of X of length k. If we number the eigenvalues of X repeated according to their multiplicities as λ_i, then a monomial of the λ_i will contribute to the spectrum of $\wedge_k X$ if and only if each λ_i appears exactly once or not at all.

[5] In [19] our so-called *exponential elements* $\mathsf{E}(X)$ are simply denoted $\Gamma(X)$ and they are related to the second quantization operator $\mathrm{d}\Gamma$

$$\mathrm{d}\Gamma(Y) := 0 \oplus Y \oplus (Y \otimes \mathbb{1} + \mathbb{1} \oplus Y)|_{\mathfrak{H}^{(2)}} \oplus \cdots$$

by the following relation

$$\Gamma(e^Y) = e^{\mathrm{d}\Gamma(Y)}.$$

We prefer not to use this notation since Γ is here also used to denote Fock spaces and generic completely positive maps. Furthermore in various other references Γ and even the term second quantization are used in a slightly different ways.

Lemma 2.2. *Exponential elements enjoy the following properties*

1. $\mathsf{E}(\mathbb{1}) = \mathbb{1}$
2. $\mathsf{E}(X)^* = \mathsf{E}(X^*)$
3. $\mathsf{E}(X)\mathsf{E}(Y) = \mathsf{E}(XY)$
4. $\mathsf{E}(X) \geq 0$ *iff* $X \geq 0$
5. $\mathsf{E}\big(X_1 \oplus X_2\big) \cong \mathsf{E}\big(X_1\big) \otimes \mathsf{E}\big(X_2\big)$
6. $\operatorname{Tr} \mathsf{E}(X) = \operatorname{Det}(\mathbb{1} + X)$
7. $\mathfrak{A}^{\mathrm{GICAR}}(\mathcal{H}) = \operatorname{Span}\big(\{\mathsf{E}(X)\}\big)$.

-

Proof. The first six statements can be easily checked by looking at the spectrum of the E-operators and properties of the graded tensor product we mentioned above. The last property follows from expanding $\lambda \mapsto \mathsf{E}(\lambda X)$ around $\lambda = 0$ and remarking that $\operatorname{Span}\big(\big\{\wedge^k X \,|\, X \in \mathcal{H}\big\}\big)$ coincides with the set of linear transformations of $\mathcal{H}^{(k)}$.

□

k-Particle projectors

Given a k-dimensional subspace $\mathcal{K}$ of $\mathcal{H}$, all vectors $\varphi_1 \wedge \cdots \wedge \varphi_k$ with $\varphi_1, \ldots, \varphi_k \in \mathcal{K}$ are proportional to each other and span therefore a one-dimensional subspace of $\mathcal{H}^{(k)}$. The projector on that space will be denoted by $\mathsf{P}_*(\mathcal{K})$. If we denote by $[\mathcal{K}]$ the projector on $\mathcal{K}$, then

$$\mathsf{P}_*(\mathcal{K}) = [\mathcal{K}] \otimes \cdots \otimes [\mathcal{K}]\Big|_{\mathcal{H}^{(k)}}.$$

It is convenient to associate the projector on the vacuum space with $\mathsf{P}_*(0)$ where 0 is the zero-dimensional vector space.

The projectors P_* are contained in the closure of $\operatorname{Span}\big(\{\mathsf{E}(X)\}\big)$ and as such inherit all relevant properties of the $\mathsf{E}(X)$ listed in lemma 2.2. They arise as the limits of normalized E-operators.

Lemma 2.3. *The projectors* P_* *arise as limits of normalized* E*-operators:*

$$\mathsf{P}_*(\mathcal{K}) = \lim_{X_n \to [\mathfrak{K}]} \operatorname{Det}(\mathbb{1} - X_n)\ \mathsf{E}\Big(\frac{X_n}{\mathbb{1} - X_n}\Big), \qquad 0 \leq X_n < \mathbb{1}.$$

-

Proof. The map $\widehat{\mathsf{E}}$ defined by

$$\widehat{\mathsf{E}}(X) \mapsto \mathrm{Det}\,(\mathbb{1} - X)\ \mathsf{E}\Big(\frac{X}{\mathbb{1} - X}\Big), \qquad 0 \leq X < \mathbb{1}$$

is uniformly continuous and extends therefore continuously to the closed interval $[0, \mathbb{1}] := \{X\ :\ 0 \leq X \leq \mathbb{1}\}$. Suppose now that 1 is a k-fold degenerate eigenvalue of X. X can then be decomposed as a direct sum of a projector P and a $(d-k)$-dimensional object,

$$X = P \oplus \tilde{X}$$

For any sequence $0 \leq (\epsilon_n)_n < 1$ that converges to 1, the operators

$$\widehat{\mathsf{E}}(\epsilon_n P \oplus \tilde{X})$$

are well defined, bounded and as per lemma 2.2 isomorphic to

$$(1-\epsilon_n)^k\,\mathrm{Det}\,(\mathbb{1} - \tilde{X})\ \mathsf{E}\Big(\frac{\epsilon_n}{1-\epsilon_n}P\Big) \otimes \mathsf{E}\Big(\frac{\tilde{X}}{\mathbb{1} - \tilde{X}}\Big).$$

By rearranging the factors in this expression, we get

$$\widehat{\mathsf{E}}(\epsilon_n P) \otimes \widehat{\mathsf{E}}(\tilde{X}).$$

We can write out the first factor as

$$(1-\epsilon_n)^k \Big\{ \Big(\bigoplus_{j \leq k} (1-\epsilon_n)^{(k-j)} \epsilon_n^j \wedge^j P \Big) \oplus \Big(\bigoplus_{j>k} 0 \Big) \Big\},$$

and then it is clear that this will converge to

$$0 \oplus \ldots 0 \oplus \big(\wedge^k P\big) \oplus 0 \ldots \oplus 0.$$

□

Remark 2.4. We will often ignore the possibility that 1 is included in the spectrum of X when we are talking about expressions containing $\widehat{\mathsf{E}}(X)$. When 1 is contained in the spectrum of X, $f\big(\widehat{\mathsf{E}}(X)\big)$ should be interpreted as

$$\lim_{X_n \to X} f\big(\widehat{\mathsf{E}}(X_n)\big), \qquad 0 \leq X_n < \mathbb{1}$$

whenever f is a continuous function.

-

Remark 2.5. We can express a general $\mathsf{E}(X)$ using the above projectors as

$$\mathsf{E}(X) = \sum_{\Lambda} x_\Lambda\, \mathsf{P}_*\big(\mathcal{H}_\Lambda\big)$$

where Λ plays the same role as in lemma 2.2 and the x_Λ are the products of the corresponding eigenvalues. So in essence, this gives us the eigendecomposition of $\mathsf{E}(X)$.

-

2.2 Quasi-free states

A linear functional ω on the CAR algebra which assigns zero values to all monomials in creation and annihilation operators except for

$$\omega\big(a^*(\varphi_1)\cdots a^*(\varphi_k)a(\psi_k)\cdots a(\psi_1)\big) = \mathrm{Det}\left(\big[\langle\psi_i\,,\,Q\,\varphi_j\rangle\big]_{i,j}\right) \tag{2.5}$$

extends to a state on $\mathfrak{A}(\mathcal{H})$ if and only if the linear one-particle space transformation Q satisfies $0 \leq Q \leq \mathbb{1}$. Such an ω is called a gauge invariant quasi-free state and Q its corresponding *symbol*. The notation ω_Q will be used to connect the state to its symbol.

The notion of quasi-free states can be extended to a larger class; the combinatorial rule (2.5) is then generalized to

$$\begin{aligned}
&\omega(\mathbb{1}) := 1\\
&\omega(c^{\#}(\varphi_1)\cdots c^{\#}(\varphi_{2n+1})) := 0\\
&\omega(c^{\#}(\varphi_1)\cdots c^{\#}(\varphi_{2n})) := \sum_p \epsilon(p)\prod_{j=1}\omega(c^{\#}(\varphi_{k_j})c^{\#}(\varphi_{l_j}))
\end{aligned} \tag{2.6}$$

In formula (2.6), the sum is taken over all ordered pair partitions p of the set $\{1,2,\ldots,2n\}$. The factor $\epsilon(p) = \pm$ depending on whether the number of crossings in the partition p is even or odd. By using an appropriate *Bogoliubov automorphism* we can always map this more general situation to a gauge-invariant one. In the following we will thus only consider the gauge-invariant case.

Using the language developed in subsection 2.1.2 we can calculate the density matrix ρ_Q corresponding to a state ω_Q.

Lemma 2.6. *The density matrix ρ_Q corresponding to a state ω_Q with symbol Q can be written down explicitly as*

$$\widehat{\mathsf{E}}(Q) = \mathrm{Det}\,(\mathbb{1}-Q)\left\{\mathbb{1}\oplus\frac{Q}{\mathbb{1}-Q}\oplus\left(\frac{Q}{\mathbb{1}-Q}\wedge\frac{Q}{\mathbb{1}-Q}\right)\oplus\ldots\right\}$$

-

Proof. Consider the symbol Q of a general quasi-free state ω. We can always find a 1D decomposition of $\mathcal{H}$ such that it is amenable with the eigendecomposition of Q, i.e.

$$Q = \sum_i q_i|e_i\rangle\langle e_i|, \qquad \mathcal{H}_i = \mathbb{C}\,|e_i\rangle\;\&\;\oplus_i\mathcal{H}_i = \mathcal{H}.$$

By straightforward computation we can check that $\omega_Q = \wedge_i\omega_{Q_i}$ with $Q_i := q_i|e_i\rangle\langle e_i|$ and since

$$\Gamma(\mathcal{H}_1\oplus\mathcal{H}_2\oplus\cdots\oplus\mathcal{H}_n) = \Gamma(\mathcal{H}_1)\otimes\Gamma(\mathcal{H}_2)\otimes\cdots\otimes\Gamma(\mathcal{H}_n),$$

$\mathfrak{A}(\oplus_i\mathcal{H}_i) \cong \otimes_i\mathfrak{A}(\mathcal{H}_i)$.

For the one-dimensional Hilbert space $\mathcal{H}_i$, the Fock space $\Gamma(\mathcal{H}_i)$ is 2-dimensional and the associated representation can be expressed on $\mathbb{C}^2$ as

$$\pi_\Gamma(a) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}; \qquad |\Omega_F\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

The relevant part of Q on this Fock space is then

$$Q_i = \begin{pmatrix} 1-q_i & 0 \\ 0 & q_i \end{pmatrix}.$$

Because of lemma 2.1 and the uniqueness implied there, the wedge state $\wedge_i \omega_{Q_i}$ must be isomorphic to the product state

$$\rho_{\tilde{Q}} = \rho_{Q_1} \otimes \ldots \otimes \rho_{Q_n}.$$

We can rewrite this in terms of exponential elements by

$$\begin{aligned} \rho_{\tilde{Q}} &= \begin{pmatrix} 1-q_1 & 0 \\ 0 & q_1 \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} 1-q_d & 0 \\ 0 & q_d \end{pmatrix} \\ &= \operatorname{Det}(\mathbb{1}-Q) \begin{pmatrix} 1 & 0 \\ 0 & \frac{q_1}{1-q_1} \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} 1 & 0 \\ 0 & \frac{q_d}{1-q_d} \end{pmatrix}, \qquad q_i \neq 1 \\ &= \operatorname{Det}(\mathbb{1}-Q)\, \mathsf{E}\left(\frac{Q_1}{\mathbb{1}-Q_1}\right) \otimes \cdots \otimes \mathsf{E}\left(\frac{Q_d}{\mathbb{1}-Q_d}\right) \end{aligned}$$

which is isomorphic to

$$\rho_Q = \operatorname{Det}(\mathbb{1}-Q)\, \mathsf{E}\left(\frac{Q}{\mathbb{1}-Q}\right).$$

Finally, by continuity of the map $\tilde{\mathsf{E}}$ this results also holds for $q_i = 1$ and so in particular for projectors.

□

By remark 2.5, there is an alternative way to write this density matrix. Let $0 \leq Q \leq \mathbb{1}$ be a linear transformation of the one-particle space $\mathcal{H}$ and let $\{e_1, e_2, \ldots, e_d\}$ be an orthonormal set of eigenvectors of Q, i.e.

$$Q\, e_j = q_j\, e_j, \qquad 0 \leq q_j \leq 1,\ j = 1, 2, \ldots, d.$$

For a subset Λ of $\{1, 2, \ldots, d\}$ define

$$q_\Lambda := \prod_{r \in \Lambda} q_r \prod_{s \in \{1,\ldots,d\}\setminus\Lambda} (1-q_s) \qquad \text{and} \qquad \mathcal{H}_\Lambda := \operatorname{Span}\big(\{e_r\,:\, r \in \Lambda\}\big)$$

then

$$\rho_Q = \sum_\Lambda q_\Lambda \, \mathsf{P}_*\big(\mathcal{H}_\Lambda\big).$$

As the $\mathsf{P}_*(\mathcal{H}_\Lambda)$ project on mutually orthogonal subspaces, this decomposition shows that the q_Λ are the eigenvalues of ρ_Q. This allows to explicitly compute quantities such as the Renyi and von Neumann entropies of ρ_Q.

As every $\mathsf{P}_*(\mathcal{K})$ defines a pure state on $\mathfrak{A}(\mathcal{H})$ that is gauge invariant and quasi-free, we see that every gauge invariant quasi-free state is a very specific convex mixture of pure gauge invariant quasi-free states. The projectors P_* are generally a small subset of the one-dimensional projectors acting on $\mathcal{H}^{(k)}$. This can be seen by a simple parameter count. In order to parameterize a generic m-dimensional complex subspace of $\mathbb{C}^n$, we need $2m(n-m)$ real parameters. As $\dim\big(\mathcal{H}^{(k)}\big) = \binom{d}{k}$ with $d = \dim(\mathcal{H})$ we need $2\big(\binom{d}{k} - 1\big)$ real parameters to specify a generic one-dimensional subspace of $\mathcal{H}^{(k)}$ that is to say a k-particle pure state on $\mathfrak{A}^{\mathrm{GICAR}}(\mathcal{H})$ while we need only $2k(d-k) \leq 2\big(\binom{d}{k} - 1\big)$ real parameters to specify a k-dimensional subspace of $\mathcal{H}$ which corresponds to a pure quasi-free state. Therefore, the convex hull of the gauge invariant quasi-free states is strictly smaller than the state space of $\mathcal{A}^{\mathrm{GICAR}}(\mathcal{H})$. The linear span of the pure quasi-free states coincides however with all linear functionals on $\mathcal{A}^{\mathrm{GICAR}}(\mathcal{H})$.

To illustrate that the quasi-free states do not form a convex set on their own, we recall the following proposition which will also be of use later on.

Proposition 2.7. *Let ω_{Q_1} and ω_{Q_2} be quasi-free and let $0 < \lambda < 1$, then $\lambda\,\omega_{Q_1} + (1-\lambda)\,\omega_{Q_2}$ is quasi-free iff $Q_1 - Q_2$ is of rank 0 or 1. Moreover, if the rank condition holds,*

$$\lambda\,\omega_{Q_1} + (1-\lambda)\,\omega_{Q_2} = \omega_{\lambda\,Q_1 + (1-\lambda)\,Q_2}.$$

-

Proof. For the proof of this we refer to [20].

□

2.2.1 Entropic measures for single site quasi-free states

The knowledge we have about the eigenvalue decomposition of a quasi-free state ω_Q allows us to translate the general expressions for entropy related quantities of that state to expressions on the one-particle density matrix.

We calculate explicitly only three types of entropies, namely the p-Renyi entropies, von Neumann entropies and the relative entropy. Other, more exotic types of entropic measures can be calculated in a similar manner. In fact, any quantity which depends only on the spectrum of a quasi-free state ρ_Q can be calculated in this fashion and reduced to a functionial on the symbol space.

Proposition 2.8. *The p-Renyi entropy of a quasi-free state ω_Q is*

$$\mathsf{H}_p(\omega_Q) = \frac{1}{1-p}\,\mathrm{Tr}\log\Big(\big(\mathbb{1}-Q\big)^p + Q^p\Big), \tag{2.7}$$

the von Neumann entropy of a quasi-free state ω_Q is

$$\mathsf{S}(\omega_Q) = -\operatorname{Tr}\Big(Q\log Q + \big(\mathbb{1}-Q\big)\log\big(\mathbb{1}-Q\big)\Big).$$

-

Proof. To prove the statement about the p-Renyi entropy $\mathsf{H}_p(\omega_Q)$,

$$\mathsf{H}_p(\omega_Q) := \frac{1}{1-p}\log\Big(\operatorname{Tr}(\rho_Q)^p\Big),$$

it suffices to use the basic properties of exponential operators in lemma 2.2,

$$\begin{aligned}
\mathsf{H}_p(\omega_Q) &= \frac{1}{1-p}\log\big(\operatorname{Tr}(\rho_Q)^p\big)\\
&= \frac{1}{1-p}\log\left[\big(\operatorname{Det}(\mathbb{1}-Q)\big)^p\ \operatorname{Tr}\left(\mathsf{E}\left(\frac{Q}{\mathbb{1}-Q}\right)\right)^p\right]\\
&= \frac{1}{1-p}\log\left[\big(\operatorname{Det}(\mathbb{1}-Q)\big)^p \operatorname{Det}\left(\mathbb{1}+\frac{Q^p}{(\mathbb{1}-Q)^p}\right)\right]\\
&= \frac{1}{1-p}\log\Big[\operatorname{Det}\Big(\big(\mathbb{1}-Q\big)^p+Q^p\Big)\Big]\\
&= \frac{1}{1-p}\operatorname{Tr}\log\Big(\big(\mathbb{1}-Q\big)^p+Q^p\Big).
\end{aligned}$$

The von Neumann entropy is the limit of the p-Renyi entropy for $p\downarrow 1$. As the expression in (2.7) becomes indeterminate $(0/0)$, we use de l'Hopital's rule combined with Jacobi's formula for differentiating a determinant

$$\frac{d}{dx}\operatorname{Det}(A) = \operatorname{Tr}\Big(A^{-1}\frac{dA}{dx}\Big)\operatorname{Det}(A).$$

This yields

$$\begin{aligned}
\mathsf{S}(\omega_Q) &= -\lim_{p\downarrow 1}\frac{d}{dp}\log\operatorname{Det}\left((\mathbb{1}-Q)^p+Q^p\right)\\
&= -\lim_{p\downarrow 1}\frac{d}{dp}\operatorname{Det}\left((\mathbb{1}-Q)^p+Q^p\right)\\
&= -\operatorname{Tr}\Big(Q\log Q+(\mathbb{1}-Q)\log(\mathbb{1}-Q)\Big).
\end{aligned}$$

□

Proposition 2.9. *Let Q_1 and Q_2 be two symbols such that $\ker Q_2\subset\ker Q_1$ and $\ker(\mathbb{1}-Q_2)\subset\ker(\mathbb{1}-Q_1)$, then the relative entropy of ω_{Q_2} with respect to ω_{Q_1} is given by*

$$\begin{aligned}
\mathsf{S}\big(\omega_{Q_1};\omega_{Q_2}\big) = \operatorname{Tr}\Big\{&Q_1\big(\log Q_1-\log Q_2\big)\\
&+(\mathbb{1}-Q_1)\big(\log(\mathbb{1}-Q_1)-\log(\mathbb{1}-Q_2)\big)\Big\}.
\end{aligned}$$

-

Proof. As above, the computation uses an appropriate limit

$$\mathsf{S}(\rho;\sigma) := \operatorname{Tr}\rho(\log\rho - \log\sigma) = \lim_{p\to 0}\frac{d}{dp}\,\operatorname{Tr}\Big(\rho^{p+1} - \rho\,\sigma^{p}\Big).$$

Using (2.7)

$$\begin{aligned}
&\mathsf{S}\big(\omega_{Q_1};\omega_{Q_2}\big)\\
&\quad= \lim_{p\to 0}\frac{d}{dp}\Big\{\operatorname{Det}(\mathbb{1}-Q_1)^{p+1}\,\operatorname{Tr}\mathsf{E}\Big(\frac{Q_1^{p+1}}{(\mathbb{1}-Q_1)^{p+1}}\Big)\\
&\qquad\qquad - \operatorname{Det}(\mathbb{1}-Q_1)\operatorname{Det}(\mathbb{1}-Q_2)^{p}\,\operatorname{Tr}\mathsf{E}\Big(\frac{Q_1}{\mathbb{1}-Q_1}\,\frac{Q_2^{p}}{(\mathbb{1}-Q_2)^{p}}\Big)\Big\}\\
&\quad= \lim_{p\to 0}\frac{d}{dp}\Big\{\operatorname{Det}\big(Q_1^{p+1}(\mathbb{1}-Q_1)^{p+1}\big) - \operatorname{Det}\big((\mathbb{1}-Q_1)(\mathbb{1}-Q_2)^{p} + Q_1Q_2^{p}\big)\Big\}\\
&\quad= \operatorname{Tr}\Big\{Q_1\big(\log Q_1 - \log Q_2\big) + (\mathbb{1}-Q_1)\big(\log(\mathbb{1}-Q_1) - \log(\mathbb{1}-Q_2)\big)\Big\}.
\end{aligned}$$

□

2.2.2 Shift invariant quasi-free states

Even if we restrict ourselves to quasi-free states, calculating entropy-like quantities becomes rather impractical if the system becomes very large. In the previous section it was explained how these calculations can be done on the level of the one particle space, but for large systems, even this space becomes too big to handle. Luckily, this can often be remediated by considering additional symmetries.

For many systems, there is a natural notion of spacial extendedness, so that we can go 'up', 'down', 'left' or 'right' in the system. On the level of the algebra, these operations are performed by special automorphisms which move observables from one part of the system to one of the neighboring parts.

Consider for instance the fermionic analogue of quantum spin chains, an infinite graded tensor product of small, identical fermionic systems,

$$\mathfrak{A}(\mathcal{H}_\infty) := \bigwedge_{i=-\infty}^{\infty}\mathfrak{A}(\mathcal{H}_i) = \mathfrak{A}\left(\bigoplus_{i=-\infty}^{\infty}\mathcal{H}_i\right), \quad \mathcal{H}_i \simeq \mathbb{C}^d.$$

We can then define an automorphism[6] α_{right} which moves operators restricted to the i^{th} subsystem to operators restricted to the $(i+1)^{th}$ subsystem. Let us first consider how this 'moving' operation comes about on the underlying one particle space $\mathcal{H}_\infty$.

[6]The dual operation α^*_{right} moves operators to the left.

We fix a basis in H_∞ which is amenable to the decomposition $\mathcal{H}_\infty = \oplus_{i=-\infty}^{\infty}\mathcal{H}_i$. For any $i \in \mathbb{Z}$ and $j \in \{1, \ldots, d\}$, we define the $(i,j)^{th}$ basis vector as

$$e_{i,j} := \left(\bigoplus_{k=-\infty}^{-i+1} 0\right) \oplus |j\rangle \oplus 0 \oplus \cdots, \tag{2.8}$$

where $|j\rangle$ is the j^{th} canonical basis vector of the Hilbert space $\mathbb{C}^d$. The operators S and S^*, defined by

$$S\, e_{i,j} = e_{(i+1),j},$$
$$S^* e_{i,j} = e_{(i-1),j},$$

are called respectively the right and left shift operator on $\mathcal{H}_\infty$. As we have seen before, such operators have a natural extension $\mathsf{E}(S)$ to the antisymmetric Fock space $\Gamma(\mathcal{H}_\infty)$ in terms of exponential elements.

We can then define the automorphism α_{right}, which moves the system to the left, in terms of these operators as

$$\alpha_{\text{right}}(X) = \mathsf{E}(S) X \mathsf{E}(S^*),$$

or equivalently on the creation and annihilation operators associated to the basis vectors $e_{i,j}$ as,

$$\alpha_{\text{right}}\left(a^*(e_{i,j})\right) = \mathsf{E}(S) a^*\left(e_{i,j}\right) \mathsf{E}(S^*) = a^*(e_{(i+1),j}).$$

Equivalently, in the Schrödinger picture, the dual[7] automorphism α^*_{right} acts on a quasi-free state as

$$\alpha^*_{\text{right}}(\rho_Q) = \mathsf{E}(S^*)\rho_Q \mathsf{E}(S) = \rho_{S^*QS},$$

Many interesting systems are invariant under this operation. For these systems, the symbol of the quasi-free states thus satisfy,

$$S^*QS = Q.$$

The structure of such a translationally invariant quasi-free state can best be understood be rewriting the one-particle operators as two-sided infinite matrices whose matrix elements are themselves d-dimensional matrices,

$$Q = [Q(k,\ell)]_{k,\ell=1-\infty}^{\infty}, \qquad Q(k,\ell) \in \mathcal{M}_d(\mathbb{C}).$$

The d-dimensional matrices $Q(k,k)$ can all be identified with reduced symbols of the k^{th} subsystem described by $\mathfrak{A}(\mathcal{H}_k)$.

Written out like this, the translation operation acts on symbols Q as

$$S^*QS = S^*[Q(k,\ell)]S = [Q(k-1,\ell-1)].$$

[7] Due to the definition of dual operations, moving operators to the right is equivalent to moving states to the left.

Since we have assumed that the state ω_Q is translation invariant,

$$Q(k,\ell) = Q(k+1,\ell+1), \qquad \forall k,\ell \in \mathbb{Z}.$$

Q is also Hermitian, so the symbols are all of the form,

$$\begin{pmatrix} \ddots & \ddots & & & \\ & Q_{11} & Q_{12} & Q_{13} & \\ & Q_{12}^* & Q_{11} & Q_{12} & \\ & Q_{13}^* & Q_{12}^* & Q_{11} & \\ & & & \ddots & \ddots \end{pmatrix}.$$

As operators, such symbols belong to the algebra $\mathcal{B}(\ell_2(\mathbb{Z},\mathbb{C}^d))$, by which we mean operators on the ℓ_2-space of sequences with elements not in $\mathbb{C}$ but $\mathbb{C}^d$. This Hilbert space is isomorphic to the set of $\mathbb{C}^d$-valued functions on the torus, parametrized by $[0,2\pi($, i.e. $\mathcal{L}^2_d(\mathbb{T},d\theta)$. An explicit isomorphism between these two spaces is provided by the Fourier transform. On the level of operators, this means that the symbol Q is unitarily equivalent with the multiplication operator $\hat{q}(\theta)$ where

$$\hat{q}(\theta) = \sum_{k\in\mathbb{Z}} q(k) e^{ik\theta},$$
$$q(k-\ell) = Q_{k,\ell}.$$

It then follows from Szegö's theorem that for any continuous function f,

$$\lim_{N\to\infty} \mathrm{Tr}_N \frac{f(Q_N)}{N} = \frac{1}{2\pi} \mathrm{Tr}_d \int_{\mathbb{T}} f(\hat{q}(\theta)) d\theta, \tag{2.9}$$

where Q_N is a restriction of Q to N sites and Tr_N the trace functional on the corresponding matrix algebra.

2.2.3 Volume scaling of entropic measures in shift invariant systems

Scaling of the von Neumann entropy

The case where the one site, one particle space is $\mathbb{C}$ has already been considered in [21]. Here we extend that result to arbitrary one site, one particle spaces. It follows directly from (2.9) that

$$\lim_{N\to\infty} \frac{\mathsf{S}(\omega_{Q_N})}{N} = \frac{1}{2\pi} \mathrm{Tr}_d \int_{\mathbb{T}} \mathsf{S}\left(\hat{q}(\theta)\right) d\theta. \tag{2.10}$$

Notice in particular that (2.10) is always a finite quantity and thus the $1/N$ is the correct scaling regime for the von Neumann entropy of a quasi-free translation invariant state.

Scaling of relative entropy

The unitary equivalence of a description in terms of multiplication operators on the torus and a description in terms of symbols also directly gives rise to a formula for the relative entropy scaling. Under the assumptions of 2.9, we obtain

$$\lim_{N\to\infty} \frac{\mathsf{S}(\omega_{Q_1};\omega_{Q_2})}{N} = \frac{1}{2\pi}\operatorname{Tr}_d \int_{\mathbb{T}} \mathsf{S}\left(\hat{q_1}(\theta);\hat{q_2}(\theta)\right) d\theta.$$

2.3 Quasi-free maps

The dynamical structure of quasi-free systems has only been partially studied [22]. As in the previous section, we will start with the historical introduction of quasi-free forms. Theorem 2.16 both extends and sharpens the maps introduced in [22] and details the structure of not only all completely positive maps, but also all plain positive maps.

Although only completely positive maps are accepted as a mathematical description of physical evolutions, plain positive maps do have their use in quantum information theory. It has recently been shown that any plain positive map can be connected to a so-called *entanglement witness*. An entanglement witness is essentially an observable which can identify in some cases whether a state is entangled or not.

In general, a single entanglement witness does not suffice to detect entanglement properly. Rather, a whole family of entanglement witnesses has to be used to verify whether a given state is entangled or not. It is a tentative question whether the set of plain positive quasi-free maps described by theorem 2.16 can be used to construct a set of entanglement witnesses powerful enough to detect any entangled state.

Heisenberg or Schrödinger

Let M be a completely positive map on $\mathcal{M}_d$. Dual to M is another completely positive map M^* on $\mathcal{M}_d$

$$\operatorname{Tr}\mathsf{M}(\sigma)\,X = \operatorname{Tr}\sigma\,\mathsf{M}^*(X), \quad \sigma, X \in \mathcal{M}_d. \tag{2.11}$$

A general quantum operation may be described either in Schrödinger or in Heisenberg picture. In the first case we use completely positive maps M with the additional property that $\operatorname{Tr}\mathsf{M}(\sigma) = \operatorname{Tr}\sigma$. Such maps restrict to affine transformations of the state space of $\mathcal{M}_d$ and are called trace-preserving completely positive (TPCP). Their duals M^* leave the identity untouched and are therefore called unity-preserving completely positive (UPCP).

2.3.1 Unital maps

We will consider here two families of UPCP maps on $\mathfrak{A}(\mathcal{H})$ which generalize the expressions for quasi-free states [22]. Any unitary U on the one-particle space $\mathcal{H}$ defines an automorphism of $\mathfrak{A}(\mathcal{H})$ through

$$a^*(\varphi) \mapsto a^*(U\,\varphi).$$

One can either check that the CAR are preserved or explicitly compute for an m-particle vector ψ

$$\begin{aligned}\mathsf{E}(U)a^*(\varphi)\mathsf{E}(U)^*\,\psi &= \mathsf{E}(U)a^*(\varphi)\,\big(\underbrace{U^*\otimes\cdots\otimes U^*}_{m\text{ times}}\,\psi\big)\\ &= \mathsf{E}(U)\varphi\wedge\big(U^*\otimes\cdots\otimes U^*\,\psi\big)\\ &= \mathsf{E}(U)\big(U^*\otimes\cdots\otimes U^*\big)\big((U\,\varphi)\wedge\psi\big)\\ &= (U\,\varphi)\wedge\psi = a^*(U\,\varphi)\psi.\end{aligned}$$

Such automorphisms are called quasi-free.

The family $\Lambda^*(A,B)$

Consider a pair A, B of linear transformations of $\mathcal{H}$ such that

$$0 \le B \le \mathbb{1} - A^*A. \tag{2.12}$$

The block matrix

$$V := \begin{pmatrix} A & \sqrt{\mathbb{1}-AA^*} \\ -\sqrt{\mathbb{1}-A^*A} & A^* \end{pmatrix}$$

is unitary on $\mathcal{H}\oplus\mathcal{H}$ and, using the constraint on (A,B), we can always find a linear map $0\le Q\le\mathbb{1}$ on $\mathcal{H}$ such that $B=\sqrt{\mathbb{1}-A^*A}Q\sqrt{\mathbb{1}-A^*A}$. Using these ingredients, we construct a UPCP map $\Lambda^*_{A,B}$ on $\mathfrak{A}(\mathcal{H})$ by concatenating three UPCP maps: the injection $a^*(\varphi)\mapsto a^*(\varphi\oplus 0)$, the quasi-free automorphism defined by the block unitary V and the projection $\mathrm{id}\wedge\omega_Q$ from $\mathfrak{A}(\mathcal{H}\oplus\mathcal{H})$ to $\mathfrak{A}(\mathcal{H})$. An explicit computation yields

$$\begin{aligned}&\Lambda^*_{A,B}\big(a^*(\varphi_1)\cdots a^*(\varphi_k)a(\psi_\ell)\cdots a(\psi_1)\big)\\ &\quad=\sum\epsilon\,\omega_B\Big(a^*(\varphi_{m_1})\cdots a^*(\varphi_{m_r})a(\psi_{n_r})\cdots a(\psi_{n_1})\Big)\\ &\qquad\times a^*(A\,\varphi_{i_1})\cdots a^*(A\,\varphi_{i_{k-r}})a(A\,\psi_{j_{\ell-r}})\cdots a(A\,\psi_{j_1}).\end{aligned}$$

Here the summation is taken over all ordered partitions

$$\Big\{\{i_1,\dots,i_{k-r}\},\{m_1,\dots,m_r\}\Big\}\quad\text{and}\quad\Big\{\{j_1,\dots,j_{\ell-r}\},\{n_1,\dots,n_r\}\Big\}$$

of $\{1,\dots,k\}$ and ϵ is the parity of the corresponding permutation.

The family $\Gamma^*(A,B)$

To define the second family, we first need a complex conjugation: fix an orthonormal basis $\{e_1, e_2, \dots, e_d\}$ in $\mathbb{C}^d$. The elements of the basis will be considered as real vectors and the complex conjugation is the conjugate linear operator J

$$J : \varphi = \sum_j c_j\, e_j \mapsto \overline{\varphi} := \sum_j \overline{c_j}\, e_j.$$

From this definition we see that $\overline{(\overline{\varphi})} = \varphi$ and $\langle \overline{\varphi}\,,\, \overline{\psi}\rangle = \langle \psi\,,\, \varphi\rangle$. We also introduce the conjugate of a complex linear transformation A by $\overline{A}\,\varphi := \overline{A\,\overline{\varphi}}$. The transformation $\overline{A}$ is complex linear and satisfies

$$\overline{A + \alpha B} = \overline{A} + \overline{\alpha}\overline{B}, \quad \overline{(\overline{A})} = A, \quad \overline{A^*} = (\overline{A})^*, \quad \text{and} \quad \overline{AB} = \overline{A}\,\overline{B}.$$

The entries of $\overline{A}$ in the distinguished basis $\{e_1, e_2, \dots, e_d\}$ are

$$(\overline{A})_{ij} = \langle e_i\,,\, \overline{A}e_j\rangle = \langle e_i\,,\, \overline{Ae_j}\rangle = \langle Ae_j\,,\, e_i\rangle = \overline{\langle e_i\,,\, Ae_j\rangle} = \overline{A_{ij}}.$$

In particular the conjugate coincides with the transpose for Hermitian elements.

The second family of maps we will consider is of the form

$$\begin{aligned}
&\Gamma^*_{A,B}\big(a^*(\varphi_1)\cdots a^*(\varphi_k)a(\psi_\ell)\cdots a(\psi_1)\big)\\
&\quad = \sum \epsilon\, \omega_B\Big(a^*(\varphi_{m_1})\cdots a^*(\varphi_{m_r})a(\psi_{n_r})\cdots a(\psi_{n_1})\Big)\\
&\qquad\qquad \times a(A\,\overline{\varphi_{i_1}})\cdots a(A\,\overline{\varphi_{i_{k-r}}})a^*(A\,\overline{\psi_{j_{\ell-r}}})\cdots a^*(A\,\overline{\psi_{j_1}})
\end{aligned}$$

with the same summation convention as above, $\Gamma^*_{A,B}$ is UPCP if and only if $0 \le B \le \mathbb{1} - A^{\mathsf{T}}(A^{\mathsf{T}})^*$.

Because we are only concerned with the action of the above maps on elements of the GICAR algebra, we could alternatively define them on the E elements. By doing this we lose something because maps defined on the GICAR algebra do not in general possess a unique extension to the CAR algebra. However the action of quasi-free maps on E elements is much easier to work with and it will turn out that even if they are not uniquely defined for the CAR, for two important subclasses demanding complete positivity is enough to uniquely extend them.

Lemma 2.10. *Suppose that $0 \le B \le \mathbb{1} - A^*A$ and $\mathbb{1} - B + XB$ invertible, then*

$$\begin{aligned}
\Lambda^*_{A,B}\big(\mathsf{E}(X)\big) &= \mathrm{Det}\,(\mathbb{1} - B + XB)\\
&\qquad \times \mathsf{E}\Big(\mathbb{1} + A(\mathbb{1} - B + XB)^{-1}(X - \mathbb{1})A^*\Big)\\
&= \mathrm{Det}\,(\mathbb{1} - B + BX)\\
&\qquad \times \mathsf{E}\Big(\mathbb{1} + A(X - \mathbb{1})(\mathbb{1} - B + BX)^{-1}A^*\Big).
\end{aligned}$$

Proof. Suppose first that $0 \leq B < \mathbb{1} - A^*A$, the general case follows by continuity. Choose now $0 \leq Q < \mathbb{1}$ and put $Q' := \gamma(Q) = A^*QA + B$, then also $0 \leq Q' < \mathbb{1}$. Recall also that the density matrix $\rho_Q = \mathrm{Det}\,(\mathbb{1} - Q)\,\mathsf{E}(Q/(\mathbb{1} - Q))$ (and the analogous expression for $\rho_{Q'}$). We now compute the action of the dual map using (2.11) and

$$\mathrm{Det}\,(\mathbb{1} + CD) = \mathrm{Det}\,(\mathbb{1} + DC), \tag{2.13}$$

$$\begin{aligned}
&\mathrm{Tr}\big(\Lambda_{A,B}(\rho_Q)\,\mathsf{E}(X)\big)\\
&\quad= \mathrm{Det}\,(\mathbb{1} - A^*QA - B)\ \mathrm{Det}\,\left(\mathbb{1} + \frac{A^*QA + B}{\mathbb{1} - A^*QA - B}X\right)\\
&\quad= \mathrm{Det}\,\big(\mathbb{1} - A^*QA - B + (A^*QA + B)X\big)\\
&\quad= \mathrm{Det}\,\big(\mathbb{1} - B + BX + A^*QA(X - \mathbb{1})\big)\\
&\quad= \mathrm{Det}\,(\mathbb{1} - B + BX)\ \mathrm{Det}\,\big(\mathbb{1} + A^*QA(X - \mathbb{1})(\mathbb{1} - B + BX)^{-1}\big)\\
&\quad= \mathrm{Det}\,(\mathbb{1} - B + BX)\ \mathrm{Det}\,\big(\mathbb{1} + QA(X - \mathbb{1})(\mathbb{1} - B + BX)^{-1}A^*\big)\\
&\quad= \mathrm{Det}\,(\mathbb{1} - B + BX)\ \mathrm{Det}\,(\mathbb{1} - Q)\\
&\qquad\times \mathrm{Det}\,\left(\frac{\mathbb{1}}{\mathbb{1} - Q} + \frac{Q}{\mathbb{1} - Q}A(X - \mathbb{1})(\mathbb{1} - B + BX)^{-1}A^*\right)\\
&\quad= \mathrm{Det}\,\left(\mathbb{1} + B(X - \mathbb{1})\right)\ \mathrm{Det}\,(\mathbb{1} - Q)\\
&\qquad\times \mathrm{Det}\,\left(\mathbb{1} + \frac{Q}{\mathbb{1} - Q}\big(\mathbb{1} + A(X - \mathbb{1})(\mathbb{1} - B + BX)^{-1}A^*\big)\right)\\
&\quad= \mathrm{Tr}\big(\rho_Q\,\Lambda^*_{A,B}(\mathsf{E}(X))\big).
\end{aligned}$$

The second form of the expression follows from (2.13) and

$$(\mathbb{1} - B + XB)^{-1}(X - \mathbb{1}) = (X - \mathbb{1})(\mathbb{1} - B + BX)^{-1}.$$

□

The maps Γ^* can be handled in a similar way.

Lemma 2.11. *Suppose that* $0 \leq B \leq \mathbb{1} - A^{\mathsf{T}}(A^{\mathsf{T}})^*$ *and that* $\mathbb{1} - B^{\mathsf{T}} - AA^* + X^{\mathsf{T}}B^{\mathsf{T}} + X^{\mathsf{T}}AA^*$ *is invertible, then*

$$\begin{aligned}
\Gamma^*_{A,B}\big(\mathsf{E}(X)\big) &= \mathrm{Det}\,\big(\mathbb{1} - B^{\mathsf{T}} - AA^* + B^{\mathsf{T}}X^{\mathsf{T}} + AA^*X^{\mathsf{T}}\big)\\
&\times\ \mathsf{E}\Big(\mathbb{1} + A(\mathbb{1} - B^{\mathsf{T}} - AA^* + X^{\mathsf{T}}B^{\mathsf{T}} + X^{\mathsf{T}}AA^*)^{-1}(\mathbb{1} - X^{\mathsf{T}})A^*\Big).
\end{aligned}$$

2.3.2 Trace-preserving maps

The stability of the set of quasi-free states with respect to quasi-free CPTP maps can essentially be used as a characterization of such maps.

Theorem 2.12. *The set of quasi-free states is invariant under a linear map* M_i *if and only if the action of the map* M_i *can be expressed as*

$$\mathsf{M}_i(\rho_Q) = \rho_{\mu_i(Q)} \tag{2.14}$$

where μ_i *is contained in one of four classes:*

$$\mu_1 = B + A^*QA \qquad \textit{where} \qquad 0 \leq B \leq \mathbb{1} - A^*A, \tag{2.15}$$

$$\mu_2 = B - A^*Q^TA \qquad \textit{where} \qquad A^*A \leq B \leq \mathbb{1}, \tag{2.16}$$

$$\mu_3 = B + A^*Q^TA \qquad \textit{where} \qquad 0 \leq B \leq \mathbb{1} - A^*A, \tag{2.17}$$

$$\mu_4 = B - A^*QA \qquad \textit{where} \qquad A^*A \leq B \leq \mathbb{1}. \tag{2.18}$$

-

Proof. Consider a map[8] $\mathsf{M} : (\mathfrak{A}^{GICAR})^* \to (\mathfrak{A}^{GICAR})^*$ with the following properties:

- trace-preserving
- $\mathbb{C}$-linear
- maps quasi-free states onto quasi-free states

Since the map M leaves the set of quasi-free states invariant, there must be a corresponding map on the set of symbols, so we propose a map μ as in (2.14). Consider now a matrix Q which is an element of the open interval $[0, \mathbb{1}[$ in $\mathfrak{M}(\mathbb{C}^d)$ and a one-dimensional projector P on the same algebra. If ϵ is small enough (but non-zero) , $Q + \epsilon P$ is still an element of the unit interval. Since the difference of Q and $Q + \epsilon P$ is of Rank 1, we can apply proposition 2.7:

$$\omega_{Q+\lambda\epsilon P} = \omega_{(1-\lambda)Q+\lambda(Q+\epsilon P)} = (1-\lambda)\omega_Q + \lambda\omega_{Q+\epsilon P}. \tag{2.19}$$

After applying the map M to (2.19) and using the linearity of M we end up with

$$\omega_{\mu(Q+\lambda\epsilon P)} = (1-\lambda)\omega_{\mu(Q)} + \lambda\,\omega_{\mu(Q+\epsilon P)}.$$

Using again proposition 2.7, this gives us the following results about μ:

$$(1-\lambda)\mu(Q) + \lambda\,\mu(Q+\epsilon P) = \mu(Q + \lambda\epsilon P) \tag{2.20}$$

[8] The * in this formula denotes the dual of the algebra, i.e. the span of the state space.

and

$$\text{Rank}\,\{\mu(Q+\epsilon P)-\mu(Q)\}=0 \quad \text{or} \quad 1\,. \tag{2.21}$$

We can rewrite (2.20) in a more useful form

$$\begin{aligned}\mu(Q+\epsilon P) &= \frac{1}{\lambda}\{\mu(Q+\lambda\epsilon P)-(1-\lambda)\mu(Q)\}\\ &= \epsilon\frac{1}{\lambda\epsilon}\{\mu(Q+\lambda\epsilon P)-\mu(Q)\}+\mu(Q)\\ &= \mu(Q)+\epsilon\, d_\lambda(Q,P)\end{aligned} \tag{2.22}$$

where in the final line we have introduced the function $d_{\lambda,\epsilon}(Q_1,Q_2)$ with the property that if Q_2 is a one-dimensional projector, the Rank of $d_{\lambda,\epsilon}$ is 0 or 1. From (2.22) we can explicitly write down two defining equation for $d_{\lambda,\epsilon}$

$$d_{\lambda,\epsilon}(Q,P) := \frac{\mu(Q+\lambda\epsilon P)-\mu(Q)}{\lambda\epsilon} \tag{2.23}$$

$$d_{\lambda,\epsilon}(Q,P) = \frac{\mu(Q+\epsilon P)-\mu(Q)}{\epsilon} \tag{2.24}$$

From (2.24) it should be clear that $d_{\lambda,\epsilon}$ actually does not depend on λ. So, the limit $\lambda\to 0$ for (2.23) exists and is equal to the directional derivative of μ at the point Q in the direction of P. Since ϵ only appears in (2.23) as a multiplicative factor of λ, the limiting operator no longer depends on the value of ϵ either and so we drop the subscripts ϵ and λ altogether.

As the maps M, $\tilde{\mathsf{E}}$ and $\tilde{\mathsf{E}}^{-1}$ are all Fréchet differentiable on the unit interval, μ should also be Fréchet differentiable. This implies that the directional derivative $d(Q,P)$ should be linear in its second argument. So clearly for any matrix $0\leq Q=\sum_i q_i P_i\leq \mathbb{1}$ such that the P_i are one-dimensional projectors,

$$\mu(Q)=\mu\left(\sum_i q_i P_i\right)=\sum_i q_i\, d(0,P_i)+\mu(0)$$

Because of the Rank conditions on $d(Q,P)$ condition, we get

$$\mu(Q)=B\pm A^*QA \qquad \text{or} \qquad \mu(Q)=B\pm A^*Q^{\mathsf{T}}A.$$

The conditions on A and B in (2.15)-(2.18) are necessary because states have to be mapped onto states, in particular the image of a symbol should remain a symbol. □

By using the relationship between trace-preserving and unital maps in (2.11), it can be easily seen that the maps $\Lambda^*_{A,B}$ and $\Gamma^*_{A,B}$ are dual to the maps induced by (2.15) and (2.16). As such, we already know these two classes to contain only completely positive maps. Complete positivity of these two classes can also be shown directly using Choi matrices. This technique also allows us to investigate whether the other two classes contain any completely positive maps.

2.3.3 Choi matrices of quasi-free maps

There is a canonical way, going by the name Jamiołkowski isomorphism, of encoding a CP map, in fact of encoding any super-operator, as a matrix $\mathsf{C}(\mathsf{M})$. Depending on the normalization and the type of map under consideration, this matrix is called either Jamiołkowksi state or Choi matrix.

Let $\{e_i\}$ be the standard basis of $\mathbb{C}^d$ with associated matrix units $e_{ij} := |e_i\rangle\langle e_j|$. The normalized Choi matrix of a linear map M is defined as

$$\mathsf{C}(\mathsf{M}) := \frac{1}{d}\sum_{ij} e_{ij} \otimes \mathsf{M}(e_{ij})\,.$$

This matrix is positive iff the corresponding map is completely positive and for trace preserving completely positive maps it is a density matrix of a state called the Jamiołkowski state.

We will compute the Choi matrix for some of the quasi-free maps introduced in theorem 2.12 and state some results on their unital duals. Since the derivation for unital maps is so similar to the trace preserving case, we omit the details of the calculations.

Proposition 2.13. *The Choi matrix of a quasi-free trace preserving map from one of the classes M_i is unitarily equivalent to a matrix $\mathsf{C} = \widehat{\mathsf{E}}(S)$.*

1. *For $M_1(\rho_Q) = \rho_{\mu_1(Q)}$ where $\mu_1(Q) = AQA^* + B$, the matrix S_1 can be written as*
$$S_1 = \frac{1}{2}\begin{pmatrix} \mathbb{1} & A \\ A^* & A^*A + 2B \end{pmatrix}.$$
2. *For $M_2(\rho_Q) = \rho_{\mu_2(Q)}$ where $\mu_2(Q) = B - A^*Q^TA$, the matrix S_2 can be written as*
$$S_2 = \frac{1}{2}\begin{pmatrix} \mathbb{1} & -A \\ -A^* & A^*A + 2B^T \end{pmatrix}.$$

-

Proof. Consider first the case of a TPCP map $\Lambda_{A,B}$. In order to stay within the context of gauge-invariant quasi-free states we embed $\mathfrak{A}(\mathcal{H})$ in the usual way in $\mathfrak{A}(\mathcal{H}\oplus\mathcal{H})$, identifying $a(\varphi)$ with $a(0\oplus\varphi)$. The gauge-invariant quasi-free state on $\mathfrak{A}(\mathcal{H}\oplus\mathcal{H})$ with symbol

$$\tfrac{1}{2}\begin{pmatrix} \mathbb{1} & \mathbb{1} \\ \mathbb{1} & \mathbb{1} \end{pmatrix} \tag{2.25}$$

is pure and its marginal on $\mathfrak{A}\big(\{0\}\oplus\mathcal{H}\big)$ is totally mixed, hence it can be used to construct the Jamiołkowski state.

The algebra $\mathfrak{A}(\mathcal{H}\oplus\mathcal{H})$ can be decomposed as $\mathfrak{A}(\mathcal{H})\otimes\mathfrak{A}(\mathcal{H})$ but the factors cannot simply be chosen as $\mathfrak{A}(\mathcal{H}\oplus 0)$ and $\mathfrak{A}(0\oplus\mathcal{H})$, indeed, $a(\varphi_1\oplus 0)$ anticommutes

with $a(0\oplus\varphi_2)$. There exists in $\mathfrak{A}(\mathcal{H})$ an element[9] Θ such that $\Theta^*=\Theta$, $\Theta^2=\mathbb{1}$ and $\{\Theta\,,\,a(\varphi)\}=0$. In fact, Θ is up to a sign uniquely defined by these requirements and using the Fock space representation of the CAR, we easily see that $\Theta=\pm\mathsf{E}(-\mathbb{1})$. Let us now embed $\mathfrak{A}(\mathcal{H})$ in $\mathfrak{A}(\mathcal{H}\oplus\mathcal{H})$ as $\imath(a(\varphi))=\Theta_1\,a(0\oplus\varphi)$ where Θ_1 is the element in $\mathfrak{A}(\mathcal{H}\oplus 0)$ just described. It is then easily checked that $\mathfrak{A}(\mathcal{H}\oplus\mathcal{H})$ decomposes into the tensor product of $\mathfrak{A}(\mathcal{H}\oplus 0)$ and the embedded algebra $\mathfrak{A}(\mathcal{H})$. Moreover,

$$\begin{aligned}\big(\mathrm{id}\otimes\Lambda^*_{A,B}\big)\big(a(\varphi_1\oplus\varphi_2)\big)&=\big(\mathrm{id}\otimes\Lambda^*_{A,B}\big)\big(a(\varphi_1\oplus 0)+a(0\oplus\varphi_2)\big)\\&=\big(\mathrm{id}\otimes\Lambda^*_{A,B}\big)\big(a(\varphi_1\oplus 0)+\Theta_1\,\Theta_1 a(0\oplus\varphi_2)\big)\\&=\big(\mathrm{id}\otimes\Lambda^*_{A,B}\big)\big(a(\varphi_1\oplus 0)+\Theta_1\otimes\imath\big(a(\varphi_2)\big)\big)\\&=\big(a(\varphi_1\oplus 0)+\Theta_1\otimes\imath\big(a(A\,\varphi_2)\big)\big)\\&=a(\varphi_1\oplus A\,\varphi_2).\end{aligned}$$

In this way, we see that $\mathrm{id}\otimes\Lambda_{A,B}$ is again quasi-free on $\mathfrak{A}(\mathcal{H}\oplus\mathcal{H})$ with defining operators

$$\tilde{A}:=\begin{pmatrix}\mathbb{1}&0\\0&A\end{pmatrix}\qquad\text{and}\qquad\tilde{B}:=\begin{pmatrix}0&0\\0&B\end{pmatrix}. \tag{2.26}$$

It is now obvious that the Jamiołkowski state will also be quasi-free with symbol

$$\begin{aligned}&\omega_{\frac{1}{2}\begin{pmatrix}\mathbb{1}&\mathbb{1}\\\mathbb{1}&\mathbb{1}\end{pmatrix}}\Big\{\big(\mathrm{id}\wedge\Lambda^*_{A,B}\big)\big(a^*(\varphi_1\oplus\varphi_2)a(\psi_1\oplus\psi_2)\big)\Big\}\\&\quad=\Big\langle\begin{pmatrix}\psi_1\\\psi_2\end{pmatrix}\,,\,\tfrac{1}{2}\begin{pmatrix}\mathbb{1}&A\\A^*&A^*A+2B\end{pmatrix}\begin{pmatrix}\varphi_1\\\varphi_2\end{pmatrix}\Big\rangle.\end{aligned}$$

Remark that the positivity conditions for the symbol of the Jamiołkowski state precisely coincide with the positivity requirement $0\le B\le\mathbb{1}-A^*A$ for the TPCP map $\Lambda_{A,B}$.

The computation for a map $\Gamma_{A,B}$ is similar. It is now convenient to compose $\mathrm{id}\wedge\Gamma_{A,B}$ with the local automorphism $\mathrm{id}\wedge\gamma$ where $\gamma(a(\varphi))=a^*(\overline{\varphi})$. In this way we remain within the class of gauge-invariant quasi-free states on the composite algebra $\mathfrak{A}(\mathcal{H}\oplus\mathcal{H})$. The extended map is now of the form $\Lambda_{\tilde{A},\tilde{B}}$ with

$$\tilde{A}:=\begin{pmatrix}\mathbb{1}&0\\0&(A^{\mathsf{T}})^*\end{pmatrix}\qquad\text{and}\qquad\tilde{B}:=\begin{pmatrix}0&0\\0&B\end{pmatrix}.$$

□

[9] Our choice of $\Theta=\mathsf{E}(-\mathbb{1})$ is often referred to in literature as the parity operator.

Choi matrix of a unital map

In order for us to compute the Choi matrix of a unital map, we first need to know how these maps act on on quasi-free states. Because of the close relationship between E-elements and quasi-free states, computing this is a simple reiteration of the proof of lemma 2.10.

Lemma 2.14. *Let Q be the symbol of a quasi-free state ω_Q and suppose that $\mathbb{1} - Q + (2Q - \mathbb{1})B$ is invertible, then*

$$\begin{aligned}\Lambda^*_{A,B}(\rho_Q) = \operatorname{Det}\big(\mathbb{1} - Q + (2Q - \mathbb{1})B\big)\\ \times \mathsf{E}\big(\mathbb{1} + A(\mathbb{1} - Q + (2Q - \mathbb{1})B)^{-1}(2Q - \mathbb{1})A^*\big).\end{aligned}$$

-

Proof. It suffices to replace X with $\frac{Q}{\mathbb{1}-Q}$ in the proof of lemma 2.10 and add the required normalization. The result also remains valid when Q becomes a projector, or even more generally, when $1 \in \sigma(Q)$ by the continuity of the map $\widehat{\mathsf{E}}$.

□

Proposition 2.15. *The Choi matrix of a quasi-free UPCP map $\Lambda^*_{A,B}$ or $\Gamma^*_{A,B}$ is unitarily equivalent to*

$$\operatorname{Det}(B)\ \mathsf{E}\Big[\begin{pmatrix} B^{-1} - \mathbb{1} & B^{-1}A^* \\ AB^{-1} & \mathbb{1} + AB^{-1}A^* \end{pmatrix}\Big]$$

for $\Lambda_{A,B}$ and

$$\operatorname{Det}(B)\ \mathsf{E}\Big[\begin{pmatrix} B^{-1} - \mathbb{1} & B^{-1}A^{\mathsf{T}} \\ (A^{\mathsf{T}})^*B^{-1} & \mathbb{1} + (A^{\mathsf{T}})^*B^{-1}A^{\mathsf{T}} \end{pmatrix}\Big]$$

for $\Gamma_{A,B}$.

-

Proof. On $\mathbb{C}^d \otimes \mathbb{C}^d$ the matrix $\sum_{ij} e_{ij} \otimes e_{ij}$ is equal to the dimension of the space times the projector on a maximally entangled vector. We should therefore compute

$$2^d\,(\mathrm{id} \wedge \Lambda^*_{A,B})\rho_Q,$$

where

$$Q = \tfrac{1}{2}\begin{pmatrix} \mathbb{1} & \mathbb{1} \\ \mathbb{1} & \mathbb{1} \end{pmatrix}.$$

Using proposition 2.14 we obtain

$$2^d \operatorname{Det}(\mathbb{1} - Q + (2Q - \mathbb{1})\tilde{B}) = \operatorname{Det}\Big[\tfrac{1}{2}\begin{pmatrix} \mathbb{1} & -\mathbb{1} \\ 2B - \mathbb{1} & \mathbb{1} \end{pmatrix}\Big] = \operatorname{Det}(B)$$

and

$$\mathbb{1} + \tilde{A}(\mathbb{1} - Q + (2Q - \mathbb{1})\tilde{B})^{-1}(2Q - \mathbb{1})(\tilde{A})^* = \begin{pmatrix} B^{-1} - \mathbb{1} & B^{-1}A^* \\ AB^{-1} & \mathbb{1} + AB^{-1}A^* \end{pmatrix},$$

where $\tilde{A}$ and $\tilde{B}$ are as in (2.26).

The computation for maps $\Gamma^*_{A,B}$ follows similar lines. Remark again that the positivity conditions for the Choi matrices coincide precisely with the conditions ensuring that $\Lambda_{A,B}$ and $\Gamma_{A,B}$ are CP.

□

2.3.4 Positive and completely positive quasi-free maps

As we mentioned in subsection 2.3.3, a linear map M is completely positive iff its Choi matrix $\mathsf{C}(\mathsf{M})$ is positive. Theorem 2.13 states that for any quasi-free preserving map the Choi matrix can be written as a normalized $\mathsf{E}(S)$-element and it is positive iff $0 \leq S \leq \mathbb{1}$. This last condition can be easily checked and so we are able to completely determine the dynamical structure of quasi-free systems.

Theorem 2.16 (structure theorem)**.** *The set of quasi-free states is invariant under a linear map M_i if and only if the action of the map M_i can be expressed as*

$$\mathsf{M}_i(\rho_Q) = \rho_{\mu_i(Q)}$$

where μ_i is contained in one of four classes:

$$\begin{aligned}
&\mu_1 = B + A^*QA && \text{where} && 0 \leq B \leq \mathbb{1} - A^*A, \\
&\mu_2 = B - A^*Q^TA && \text{where} && A^*A \leq B \leq \mathbb{1}, \\
&\mu_3 = B + A^*Q^TA && \text{where} && 0 \leq B \leq \mathbb{1} - A^*A, \\
&\mu_4 = B - A^*QA && \text{where} && A^*A \leq B \leq \mathbb{1}.
\end{aligned}$$

A map M_i is completely positive *if μ_i belongs to any of two classes*

$$\begin{aligned}
&\mu_1 = B + A^*QA && \text{where} && 0 \leq B \leq \mathbb{1} - A^*A, \\
&\mu_2 = B - A^*Q^TA && \text{where} && A^*A \leq B \leq \mathbb{1}.
\end{aligned}$$

-

2.4 Discussion

The analysis of the behavior of a quantum system is typically hampered by the complicated correlations which can arise in such a system. In many cases, considering the physical symmetries of a quantum system can bring some relief. In

particular, if a system can be said to be composed entirely of identical fermionic particles, the Pauli exclusion principle places bounds on the possible correlations which can arise in such a system.

In such fermionic system, the interaction between different particles is often dominated by this Pauli exclusion principle and the quasi-free approximation is warranted. The quasi-free approximation reduces again the possible correlations in the system and in effect simplifies the description of such systems exponentially.

The main physical results described in this chapter are the reduced formulas for the various entropic measures in section 2.2 and the full characterization of quasi-free completely positive and plain positive maps in theorem 2.16.

As the mathematical representations of physical evolutions, the quasi-free completely positive maps should be useful to investigations on the structure of dynamical fermionic systems. At the time of publication of this thesis, they have already proven their usefulness in several research papers, for instance [23, 24, 25].

The usefulness of plain positive quasi-free maps is more tentative. As it was explained in this chapter, plain positive maps can be used to construct entanglement witnesses, observables which can identify a state as being entangled or not. It is an open question whether the quasi-free plain positive maps can be used to construct a complete family of entanglement witnesses. And if not, what type of entangled states *can* be detected by such quasi-free entanglement witnesses.

Finally, we would like to motivate the use of the exponential elements in describing quasi-free systems. They are useful not only because they make the calculation of the various entropy measures almost trivial, but they are also the natural observables to define the action of a quasi-free map on. The E-elements form an invariant set for all maps described by our structure theorem 2.12 and the image of quasi-free maps on an E-element is again a single E-element. In contrast, the image on monomials of creation and annihilation operators is a very large sum over monomials in creation and annihilation operators, from which no physical intuition can be gleaned on what the quasi-free map actually does.

CHAPTER 3

The power of being free

> If you want to be free, there is but one way; it is to guarantee an equally full measure of liberty to all your neighbors. There is no other.
>
> Carl Shurz

The notion of independent random variables, although not quite yet taught at elementary school, is probably one of the best-studied concepts in any[1] introductory statistics course. It owes its popularity both to the implied simplicity in dealing with multiple random variables and the wide range of established applications in mathematics, physics, economics, biology, and almost any other field where some form of stochasticity is present.

The non-commutative analogues of independent random variables , *free random variables*, are rather less well-known[2], but certainly not less interesting nor lacking in potential applications [27, 28, 29, 30, 31, 32, 33, 34]. Although it may not be directly clear from the definition of freeness in section 3.2, the joint distribution of multiple free random variables is determined in full by the distribution of the individual free random variables, not unlike the way independence dictates how the joint distribution of independent random variables behaves. In many cases, this significantly simplifies calculations and so it can be a great tool for the lazy physicist.

[1] We used Google's PageRank [26] system to compile a set of 5 popular introductory books on statistics. If we use the page rank of links related to these books to compute a normalized distribution for these books, then we find that the concept of independent random variables is almost surely introduced by page 4. As such, it probably didn't need an introduction in this text.

[2] A short survey taken among PhD students at the Institute for Theoretical Physics of the KULeuven showed only one in ten was knowledgeable about the subject.

The theory of free random variables, known to mathematicians [35, 36, 37] and Google as 'free probability theory', was founded by Voiculescu [38] in the 1980's. Although he originally intended it as a research tool to investigate free group factors, it soon branched out in wildly different and unsuspected directions. One being the connection to random matrices, which is the motivation for using free probability in chapter 4.

In the limit of infinite dimensional matrix algebras, matrices drawn from unitarily invariant random matrix ensembles [39, 40] behave like free random variables, both in terms of the algebraic operations permitted on matrices and in the behavior of their empirical and mean eigenvalue density. So instead of manipulating ensembles of very large numerical random matrices, we can use the algebraic description of free random variables.

Because of its origin, Voiculescu's original description is phrased in the language of group von Neumann algebras, which is perhaps a bit heavy-handed for our purposes. A complementary description of free probability, based on *non-crossing cumulants*, was developed by Speicher [41, 42, 36, 43]. It highlights the combinatorial nature of freeness and translates perhaps more clearly that, like independent random variables, free random variables have a rather carefree attitude when dealing with multiple random variables. This is evident in the additivity of non-crossing cumulants for sums of free random variables, similar to how classical ordered cumulants behave under addition of independent random variables. Non-crossing cumulants also give rise to a non-commutative analogue of the second characteristic function[3] called the *free cumulant series*, which retains additivity for sums of free random variables and an associated *free convolution* which describes the probability measure of sums of free random variables.

This chapter is intended as a crash course in free probability; it covers but a fraction of the theoretical underpinnings of Voiculescu's beautiful theory. Only the concepts needed for the model-specific calculations in chapter 4 are introduced and by necessity the current chapter also lacks some rigor. A complete and rigorous description of free probability would require an introduction of mathematics which is far beyond the length- and timescale of this thesis.

Free probability theory, at least in the form it is presented in this chapter, does not lend itself very well to explicit computations or numerical approximations, a deficit that has only recently started to receive some attention [44, 45, 46, 47, 48, 49]. This was a major hurdle in tackling the type of questions posed in chapter 4 and so new techniques had to be developed. These techniques have applications beyond the physical picture in which they are introduced and especially the numerical approximation scheme introduced in chapter 4 can be used to model any system composed of free random variables. We hope that the explanation of these techniques in the following chapter can make up for the terseness of the exposition in this chapter.

[3]The second characteristic function is alternatively called the cumulant generating function when considering classical cumulants.

Bounding our box

For the remainder of this chapter, we will assume that we are dealing with bounded hermitian operators. This is not a crucial point for the calculations in this chapter or in chapter 4, as most can be easily resumed in a more general setting with unbounded normal operators. It is a mostly cosmetic choice to restrict ourselves to the bounded case.

A word on notation

In the following, we have tried to adhere to the notation and nomenclature[4] as presented in [41]. Towards the end of this chapter, when we introduce the *cumulant series* (definition 3.32), we stray a little from that path. Our cumulant series is alternatively called R-series or R-transform in various references and both the terms R-series and R-transform can be found in any given reference, but refer to different mathematical objects. To avoid any confusion when comparing results presented here with the literature on free probability, we have opted to use the more neutral term, cumulant series.

3.1 Non-commutative probability spaces

In classical probability theory, the concept of a random variable is usually presented from a phenomenological point of view. In a handpicked set of experiments or situations, random variables are introduced, defined or described as objects not with a definite value, but rather, objects which can take any value in a predetermined set of outcomes with a probability of occurrence associated to each possible outcome. After this, the mathematical context of Kolmogorov probability spaces is described which fits this intuitive notion of what a random variable is.

To transplant the notion of random variables to a quantum setting, we will go the other way around and define random variables ad hoc and then look at specific situations where these might arise. As a bonus, this allows a straightforward but important generalization from what is usually considered in probability textbooks: the notion of *operator-valued* random variables; which are roughly speaking regular random variables which take values not in $\mathbb{R}$ or $\mathbb{C}$, but in a general algebra $\mathcal{B}$.

Definition 3.1 (non-commutative probability spaces)**.**

1. Let $\mathcal{A}$ be a C^*-algebra and $\mathcal{B}$ a subalgebra of $\mathcal{A}$. A linear map $\mathbb{E} : \mathcal{A} \to \mathcal{B}$ is called a *conditional expectation* onto $\mathcal{B}$ if

   (a) $\mathbb{E}$ is completely positive,

   (b) $\mathbb{E}[b_1 a b_2] = b_1 \mathbb{E}[a] b_2$ for all $b_1, b_2 \in \mathcal{B}$ and $a \in \mathcal{A}$,

[4] As a consequence, most definitions are a rephrasing of the definitions found there and may seem rather convoluted or excessively detailed.

(c) $\mathbb{E}\left[\mathbb{1}_{\mathcal{A}}\right] = \mathbb{1}_{\mathcal{B}}$.

2. A pair $(\mathcal{A}, \mathbb{E})$, consisting of a C^*-algebra $\mathcal{A}$ with a unital subalgebra $\mathcal{B}$ and a conditional expectation $\mathbb{E} : \mathcal{A} \mapsto \mathcal{B}$ is called a *probability space* (over $\mathcal{B}$).

3. Given a probability space $(\mathcal{A}, \mathbb{E})$ over $\mathcal{B}$, an element $a \in \mathcal{A}$ is called a $\mathcal{B}$-*valued random variable*, with notation $a \in (\mathcal{A}, \mathbb{E})$.

4. For any random variable a, we call $\mathbb{E}\left[a\right]$ the *(conditional) expectation of* a. If $\mathcal{B} = \mathbb{C}$, we call $\mathbb{E}\left[a\right]$ the *expectation value of* a.

-

3.1.1 Random variables in quantum mechanics

A modern description of a quantum mechanical system requires a so-called dynamical triple $(\mathcal{A}, \omega, \alpha_t)$ where $\mathcal{A}$ is a C^*-algebra that contains all observables of the system as Hermitian operators, ω is a state of the system and α_t is a time-dependent completely positive map on the algebra $\mathcal{A}$ expressing the time evolution of the system. In quantum information theory, the role of the state ω is often subsumed by the introduction of a density matrix $\rho \in \mathcal{A}$ such that

$$\mathrm{Tr}\, \rho\, a = \omega(a), \qquad \forall a \in \mathcal{A}.$$

For the moment we wil also assume that the system A undergoes a Hamiltonian evolution, i.e.

$$\alpha_t(a) = e^{-itH} a\, e^{itH}, \qquad \forall a \in \mathcal{A},$$

or equivalently in the Schrödinger picture,

$$\omega_t(a) = \mathrm{Tr}\left[\left(e^{itH} \rho\, e^{-itH}\right) a\right], \qquad \forall a \in \mathcal{A}.$$

In many applications, one is not interested in a description of the entire system, but only in knowing the expectation value of a small subset of observables $\mathcal{S}$, localized in space-time or in some other way delineated from the rest of the system. From a pragmatic point of view, $\mathcal{S}$ is usually associated to the degrees of freedom an experimentator would be able to control or measure. For instance, for a single spin 1/2 particle, these might be the position, speed and spin of the particle.

The remaining degrees of freedom are put in a, sometimes hypothetical, environment $\mathcal{E}$ such that $\mathcal{A}$ is a subalgebra of $\mathcal{S} \otimes \mathcal{E}$. As far as experiments go, this environment is usually inaccessible to the experimentator, except for some macroscopic observables, such as temperature, pressure, ...

The description of quantum systems in terms of a dynamical triple is flexible enough to also allow for such a reduced description, i.e. we can find a state $\tilde{\omega}$ and dynamical mapping $\tilde{\alpha}_t$ defined for the algebra $\mathcal{S}$ such that

$$\omega\Big(\alpha_t(x \otimes \mathbb{1})\Big) = \tilde{\omega}\Big(\tilde{\alpha}_t(x)\Big), \qquad \forall\, x \in \mathcal{S}.$$

The connection between these two descriptions is most easily made by introducing a conditional expectation $\mathbb{E}$ as in definition 3.1. The trace Tr over the system $\mathcal{A}$ can be written as the joint application of the trace Tr_S over the system $\mathcal{S}$ and the trace Tr_E over the environment $\mathcal{E}$,

$$\mathrm{Tr}[a] = (\mathrm{Tr}_S \otimes \mathrm{Tr}_E)[a] = \mathrm{Tr}_S\Big[(\mathrm{id} \otimes \mathrm{Tr}_E)[a]\Big], \quad \forall a \in \mathcal{A}.$$

For the state ω and an observable $x \in \mathcal{S}$, we can use this to come up with a reduced description,

$$\mathrm{Tr}\,\rho\,(x \otimes \mathbb{1}) = \mathrm{Tr}_S\Big[(\mathrm{id} \otimes \mathrm{Tr}_E)[\rho]\,x\Big].$$

It is a straightforward calculation to see that the map

$$\mathbb{E} : a \mapsto (\mathrm{id} \otimes \mathrm{Tr}_E)[\rho\, a]$$

is a conditional expectation from $\mathcal{S} \otimes \mathcal{E}$ to $\mathcal{S}$. It is also compatible with the states ω and $\tilde{\omega}$ in the sense that

$$\omega(a) = \tilde{\omega}\left(\mathbb{E}\left[a\right]\right), \quad \forall\, a \in \mathcal{A}.$$

In particular, this can be used to construct a reduced dynamics for the system $\mathcal{S}$,

$$\tilde{\alpha}_t(x) := \mathbb{E}\left[\alpha_t(x \otimes \mathbb{1})\right], \quad \forall\, x \in \mathcal{S}.$$

3.1.2 Distributions and probability measures

Above, it was established how we can introduce the concept of random variables in quantum mechanics by considering reduced descriptions of dynamical quantum systems. The construction we used still relies on a description of the complete quantum system $\mathcal{A}$ to determine the dynamics of the reduced system $\mathcal{S}$. However, a description of the reduced system $\mathcal{S}$ should require less information than a description of the system $\mathcal{A}$. The projection of the system $\mathcal{A}$ onto the subsystem $\mathcal{S}$ effectively reduces the amount of information an observer can extract. How do we now determine the minimal amount of information about the complete system $\mathcal{A}$ that we need in order to construct the dynamical triple for the system $\mathcal{S}$?

In commutative probability theory, the distribution of a random variable a is defined as a sequence ν_a containing the expectation values of all powers of a.

$$\nu_a = \Big(\mathbb{E}\left[a\right], \mathbb{E}\left[a^2\right], \ldots\Big).$$

This information suffices to calculate the expectation value of any holomorphic function of a by writing the function f as a Taylor series,

$$\mathbb{E}\left[f(a)\right] = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!}\, \mathbb{E}\left[a^n\right].$$

Similarly, all probabilistic information about an operator-valued random variable is encoded in its distribution. However, the distribution of an operator-valued random variable contains a lot more information than its classical cousin.

Consider the situation of section 3.1.1 for a random variable $a \in \mathcal{S} \otimes \mathcal{E}$ and observables b_1 and $b_2 \in \mathcal{S}$. Linearity of the conditional expectation $\mathbb{E}$ allows us to calculate $\mathbb{E}\left[(b_1 \otimes \mathbb{1})\, a^2\, (b_2 \otimes \mathbb{1})\right]$ from the knowledge of $\mathbb{E}\left[a^2\right]$, b_1 and b_2 alone. Indeed,

$$\mathbb{E}\left[(b_1 \otimes \mathbb{1})\, a^2\, (b_2 \otimes \mathbb{1})\right] = b_1 \mathbb{E}\left[a^2\right] b_2.$$

However, if we wish to calculate $\mathbb{E}\left[a(b_1 \otimes \mathbb{1})a(b_2 \otimes \mathbb{1})\right]$, we need more information, since

$$\mathbb{E}\left[a(b_1 \otimes \mathbb{1})a(b_2 \otimes \mathbb{1})\right] = \mathbb{E}\left[a(b_1 \otimes \mathbb{1})a\right] b_2.$$

Without knowledge of the commutation relations between $b_1 \otimes \mathbb{1}$ and a, we cannot work out $\mathbb{E}\left[a(b_1 \otimes \mathbb{1})a\right]$ any further and both $\mathbb{E}\left[a^2\right]$ and $\mathbb{E}\left[a(b_1 \otimes \mathbb{1})a\right]$ contribute information to the distribution of a.

Definition 3.2. Let $\mathcal{B}\langle X\rangle$ be the algebra freely generated by $\mathcal{B}$ and an indeterminate X, i.e. the algebra composed of linear combinations of finite words containing elements $b_i \in \mathcal{B}$ and the indeterminate X, e.g.

$$b_1 X b_2 X X X b_1 X X b_3 \cdots X b_n.$$

For a probability space $(\mathcal{A}, \mathbb{E})$ over $\mathcal{B}$ and a random variable $a \in (\mathcal{A}, \mathbb{E})$, we define the $\mathcal{B}$-functional,

$$\nu_a : \mathcal{B}\langle X\rangle \to \mathcal{B} \qquad \text{by} \qquad \nu_a := \mathbb{E} \circ \tau_a,$$

where $\tau_a : \mathcal{B}\langle X\rangle \to A$ is the unique homomorphism such that $\tau_a(b) = b$ for all $b \in \mathcal{B}$ and $\tau_a(X) = a$. ν_a is called the *distribution* of the random variable a.

-

Remark 3.3. The additional abstraction of introducing $\mathcal{B}\langle X\rangle$ instead of defining a distribution ν'_a directly on the algebra $\mathcal{A}$ may seem a little contrived. In specific cases this can certainly be true, but when considering less well behaved random variables, e.g. unbounded, non-normal operators, this level of abstraction removes any worries about boundedness or convergence. When considering multiple random variables, this also allows us to treat distributions of different random variables on an equal footing.

-

Scalar-valued random variables

For scalar-valued Hermitian random variables, $\mathcal{B} = \mathbb{R}$ and $\mathcal{B}\langle X\rangle$ is just the algebra containing all possible polynomials in the indeterminate X. The Riesz-Markov

theorem [50] then states that there exists a unique measure μ_a on $\mathbb{R}$ such that

$$\nu_a\left(f(X)\right) = \int_{-\infty}^{+\infty} f(x)\,\mu_a(dx), \qquad \forall f \in \mathbb{R}\langle X\rangle. \tag{3.1}$$

μ_a summarizes all the information contained in the distribution of a and is called the *probability measure* of a.

Definition 3.4. If a function $\rho : \mathbb{R} \to \mathbb{R}^+$ exists such that

$$\nu_a(f(X)) = \int_{-\infty}^{+\infty} f(x)\rho(x)dx, \qquad \forall f \in \mathbb{R}\langle X\rangle,$$

we call $\rho(x)$ the *probability density function* of a. The Fourier transform $\chi(y)$

$$\chi(y) = \frac{1}{2\pi i}\int_{-\infty}^{+\infty} e^{iyx}\rho(x)dx = \mathbb{E}\left[e^{iya}\right]$$

of $\rho(x)$ is called the *moment generating function*[5] of a.

-

Example 3.5 (the semicircle distribution)**.** Some of the most celebrated distributions in free probability theory are the semicircle laws. Their probability density functions $w_{m,v}$ are,

$$w_{m,v}(x) = \begin{cases} \frac{2}{\pi v^2}\sqrt{v^2-(x-m)^2} & \text{if } m-v \le x \le m+v, \\ 0 & \text{otherwise,} \end{cases}$$

where m and r are real numbers and $r > 0$. m is the mean, or expectation value of the semicircle distribution and $v^2/4$ the variance. If $m = 0$ and $v = 2$, then the corresponding semicircle law is called standard. The moments m_n of this distribution are

$$m_n = \begin{cases} 0 & \text{if n=2 k+1,} \\ \frac{1}{k+1}\binom{2k}{k} & \text{if } n = 2k. \end{cases}$$

The numbers $C_k = \frac{1}{k+1}\binom{2k}{k}$ are called the Catalan numbers.

-

[5] Alternatively, this function is also called the first characteristic function of a.

Operator-valued random variables

The concept of a probability density function can be generalized to operator-valued random variables. Given a normal operator $a \in \mathcal{A}$, a von Neumann algebra, the spectral theorem states that there exists a unique projection-valued measure M on the complex plane $\mathbb{C}$ such that

$$a = \int_{\Sigma(a)} z\, M(dz),$$
$$f(a, a^*) = \int_{\Sigma(a)} f(z, \overline{z})\, M(dz), \qquad \forall f \text{ continuous},$$

where integration with respect to the projection-valued measure may be understood as

$$\varphi\big(f(a, a^*)\big) = \int f(z, \overline{z})\, \varphi\big(M(dz)\big)$$

for every $\varphi \in \mathcal{S}(A)$, the state space of algebra $\mathcal{A}$. The complex-valued measure μ_φ, defined by

$$\mu_\varphi : Y \mapsto \varphi(M(Y)), \qquad Y \subset \mathbb{C},$$

is the probability measure as introduced in (3.1).

Similarly, if the state φ in equation (3.1.2) is replaced by a conditional expectation $\mathbb{E}$ onto a unital algebra $\mathcal{B}$, the spectral theorem states that

$$\mathbb{E}\big(f(a, a^*)\big) = \int f(z, \overline{z})\, \mathbb{E}\big(M(dz)\big),$$

and an *operator-valued probability measure* μ_a of X under $\mathbb{E}$ can be defined as

$$\mu_a : Y \mapsto \mathbb{E}\big(M(Y)\big), \qquad Y \subset \mathbb{C}.$$

The operator-valued versions of the probability density function and moment generating function are defined analogously to definition 3.4.

It should be noted that in this case the probability measure of a random variable contains strictly less information than the distribution. In the non-commutative case, a generic element in $\mathcal{B}\langle X\rangle$ is a linear combination of

$$b_0 X b_1 X \cdots X b_n, \qquad n \in \mathbb{N}, \tag{3.2}$$

but no useful commutation relation between X and the b_i exists and therefore the expectation of (3.2) cannot be calculated from the probability measure μ_a alone.

3.1.3 Joint distributions

Definition 3.6. Let $B\langle X_1, \ldots, X_m\rangle$ be the algebra freely generated by B and m non-commuting (self-adjoint) indeterminates $X_1, \ldots, X_m$. For a probability

space $(\mathcal{A}, \mathbb{E})$ over $\mathcal{B}$ and m random variables $a_1, \ldots, a_m \in (\mathcal{A}, \mathbb{E})$ we define the $\mathcal{B}$-functional

$$\nu_{(a_1,\ldots a_m)} : \mathcal{B}\langle X_1, \ldots, X_m\rangle \to B \qquad \text{by} \qquad \nu_{(a_1,\ldots,a_m)} := \mathbb{E} \circ \tau_{(a_1,\ldots,a_m)}, \tag{3.3}$$

where $\tau_{(a_1,\ldots,a_m)} : \mathcal{B}\langle X_1, \ldots X_m\rangle \to \mathcal{A}$ is the unique homomorphism such that $\tau_{(a_1,\ldots,a_m)}(b) = b$ for all $b \in \mathcal{B}$ and $\tau_{(a_1,\ldots,a_m)}(X_i) = a_i$ for all $i = 1, \ldots, m$. $\nu_{(a_1,\ldots,a_m)}$ is called the *joint distribution* of the random variables $a_1, \ldots, a_m$.

-

Example 3.7 (joint scalar probability measures)**.** As in the case of a single scalar random variable, for a set of m commuting scalar random variables we can construct a *(joint) probability measure on* $\mathbb{C}^m$ such that $\forall f \in \mathbb{C}\langle X_1, \ldots, X_m\rangle$,

$$\nu_{(a_1,\ldots,a_m)}\left(f(X_1, \ldots, X_m)\right) = \int_{\mathbb{C}^m} f(x_1, \ldots x_m) d\mu(x_1, \ldots, x_n).$$

-

Already in the simple example 3.7 it can be seen that a joint probability measure is a hugely more complicated object than the probability measure of a single random variable. It details not only all moments of a single random variable, but also contains all information on correlations between different random variables.

Only in a few, very select cases does it become feasible to actually compute or determine the joint probability measure of several random variables. The most well-known case is without a doubt a system of independent random variables.

Definition 3.8 (independent random variables)**.** Let $(\mathcal{A}, \mathbb{E})$ be a probability space and $\mathcal{A}_1, \mathcal{A}_2 \subset \mathcal{A}$. The algebras A_1 and A_2 are called *independent (with respect to* $\mathbb{E}$*)* if for all $a_1 \in \mathcal{A}_1$ and $a_2 \in \mathcal{A}_2$, $a_1 a_2 = a_2 a_1$ and

$$\mathbb{E}\left[a_1 a_2\right] = \mathbb{E}\left[a_1\right] \mathbb{E}\left[a_2\right]. \tag{3.4}$$

If $\mathcal{A}_1$ and $\mathcal{A}_2$ are independent, then any $a_1 \in \mathcal{A}_1$ and $a_2 \in \mathcal{A}_2$ are also called *independent*.

-

Remark 3.9. It can easily be seen that independence implies that the outcomes or expectation values of different random variables are not conditioned upon each other. Often, this observation is taken as the defining property of independent random variables. This is actually not correct. There are several types of random variables which also have this property, but are *not* independent. In particular, free random variables, which we will introduce in the next section, do not commute, but their outcomes also cannot be conditioned upon each other.

-

Example 3.10 (probability measures of independent random variables)**.** As we have seen, the Riesz-Markov theorem can be used to construct meaures μ_{a_i} such that

$$\nu_{a_i}\left(f(X_i)\right) = \int_{\mathbb{C}} f(x_i)\mu_{a_i}(dx), \qquad \forall f \in \mathbb{C}\langle X_i\rangle.$$

In the case of independent a_i, the joint probability measure $\mu_{a_1,\ldots,a_m}$ appearing in example 3.7 can be rewritten in terms of these measures μ_{a_i},

$$\nu_{(a_1,\ldots,a_m)}\left(f(X_1,\ldots,X_m)\right) = \int_{\mathbb{C}^m} f(x_1,\ldots,x_m).\prod_{i=1}^{m}\mu_{a_i}(dx_i) \tag{3.5}$$

-

Example 3.11 (Classical convolution)**.** If one is only interested in the sum of two independent random variables (a_1+a_2), a measure $\mu_{a_1+a_2}$ on $\mathbb{C}$ can be constructed, which is the probability measure of the sum (a_1+a_2),

$$\nu_{(a_1,a_2)}\left(f(X_1+X_2)\right) = \nu_{a_1+a_2}\left(f(X)\right) = \int_{\mathbb{C}} f(x)\mu_{a_1+a_2}(dx), \qquad \forall f \in \mathbb{C}\langle X\rangle,$$

where $\mu_{a_1+a_2} = \mu_{a_1} * \mu_{a_2}$, the usual convolution of μ_{a_1} and μ_{a_2}. The first characteristic function of the sum is the product of the characteristic functions of a_1 and a_2.

-

3.2 What does it mean to be free?

As we mentioned in the introduction of this chapter, there exists a non-commutative *analogue* of independent random variables, namely free random variables. Not only does this reduce the complexity of multivariate distributions in a similar way as independence does, but it will also allow us to rewrite probability measures for sums[6] of free random variables in terms of the probability measures of the individual random variables using an operation called *free convolution*. This will be the main point of section 3.4. Here we focus on some elementary properties of free random variables, illustrated by a few select examples.

Definition 3.12 (free algebras)**.**

1. Let $(\mathcal{A},\mathbb{E})$ be a probability space over $\mathcal{B}$ and $\mathcal{A}_1,\ldots,\mathcal{A}_m$ unital subalgebras. $\mathcal{A}_1,\ldots,\mathcal{A}_m$ are called *free (with amalgamation over $\mathcal{B}$)* if

$$\forall\, n \in \mathbb{N},\, \forall\, a_i \in \mathcal{A}_{k(i)}, \quad 1 \le i \le n, \text{ and } k(i)) \neq k(i+1),$$

[6] An analogue procedure as the one we will follow here, also allows to treat products of free random variables.

$$\mathbb{E}\left[a_1 a_2 \cdots a_n\right] = 0,$$

if for all i,

$$\mathbb{E}\left[a_i\right] = 0.$$

2. If $\mathcal{A}_1, \ldots, \mathcal{A}_m$ are free with amalgamation over $\mathcal{B}$, then the set $(a_i)_{i=1,\ldots,m}$ with $a_i \in \mathcal{A}_i$ is also called *free with amalgamation over* $\mathcal{B}$.

-

Example 3.13 (random subsystems)**.** Suppose we have a more or less uniform system, such as a quantum gas, but we are only interested in the interaction between two randomly chosen parts of that gas to study for instance the correlation length in the system. For a single subsystem, we can simple project the global system using a projector such as P_n. To choose a second subsystem, we need an appropriate notion of randomness. The simplest such notion is derived from the structure of $U(2n)$, the group of unitary transformations of $\mathcal{H}_{2n}$. This group admits a natural two-sided invariant measure, called the Haar measure μ. The key feature of this measure is that is translation invariant with regards to the group operations and thus it assigns weights uniformly. Using this measure μ we can construct a random projector Q_n by picking a random unitary, U, according to the measure μ from the group $\mathcal{U}_{2n}$ and rotating the projector P_n over this unitary U,

$$Q_n = U P_n U^*.$$

It is then a standard result in free probability theory that in the limit $n \to \infty$, $P = \lim P_n$ and $Q = \lim Q_n$ will be free over $\mathbb{C}$ in the probability space $(\mathcal{B}(\mathcal{H}), \tau)$ where τ is the normalized trace functional. The ranges of Q and P are then also referred to as random subsystems.

This may seem a rather abstract result, but it is exactly this type of reasoning which leads to the identification between free random variables and infinite dimensional unitarily invariant random matrices. We will discuss this identification further in section 3.5.

We will show how the spectrum of the sum of two free random variables can be computed in theorem 3.34. After this theorem, we will come back to this example and show how we can calculate the spectrum of $P + Q$.

-

Example 3.14 (Constants are free from everything)**.** *Consider a probability space* $(\mathcal{A}, \mathbb{E})$ *over* $\mathcal{B}$*. The algebras* $\mathcal{A}$ *and* $\mathcal{B}$ *are free with amalgamation over* $\mathcal{B}$*.*

We should check whether an expression of the form

$$\mathbb{E}\left[a_1 b_1 a_2 b_2 \cdots a_n b_n\right] \stackrel{?}{=} 0, \qquad \text{where } a_i \in \mathcal{A},\ b_i \in \mathcal{B}, \tag{3.6}$$

if

$$\mathbb{E}\left[a_i\right] = 0 \quad \text{and} \quad \mathbb{E}\left[b_i\right] = 0. \tag{3.7}$$

Since $\mathbb{E}[b_i] = b_i$,

$$\mathbb{E}[b_i] = 0 \text{ iff } b_i = 0.$$

So, if (3.7) is true, then (3.6) is equal to

$$\mathbb{E}[a_1 0 a_2 0 \cdots a_n 0] = 0,$$

and we see that $\mathcal{A}$ is free from $\mathcal{B}$ with amalgamation over $\mathcal{B}$.

-

As promised, definition 3.12 can be used to compute expectation values of words containing any number of free random variables. Consider for instance the monomial $a_1 a_2 \cdots a_n$, where the a_i are free (with amalgamation over some $\mathcal{B}$). We would like to know

$$\mathbb{E}[a_1 \cdots a_n].$$

Since the a_i are free, we know that

$$\mathbb{E}\big[\big(a_1 - \mathbb{E}[a_1]\big)\big(a_2 - \mathbb{E}[a_2]\big) \cdots \big(a_n - \mathbb{E}[a_n]\big)\big] = 0. \tag{3.8}$$

$\mathbb{E}$ is linear, so we can expand out the differences appearing in this expression. Only one of the terms in this expansion is the expectation of a monomial of length n, all others are of lower order. We can use this identity to rewrite (3.8) in terms of shorter monomials,

$$\mathbb{E}[a_1 \cdots a_n] = \sum_{r=1}^{n} \sum_{1 \le k_1 < \ldots k_r < n} (-1)^{r+1} \mathbb{E}\big[a_1 \cdots a_{k_j - 1} \mathbb{E}\left[a_{k_j}\right] a_{k_j + 1} \cdots X_n\big].$$

This scheme can be continued until all expectations are reduced to expectations of a single random variable and operators from $\mathcal{B}$. It is important to remark that freeness with amalgamation over a subalgebra $\mathcal{B}$ only reduced expectations of random variables up to elements of $\mathcal{B}$, i.e. expressions of the form

$$\mathbb{E}[a_i b_1 a_i b_2 \cdots a_i], \qquad \forall k,\, b_k \in \mathcal{B}.$$

Such expressions can be calculated from the knowledge of the distribution of a_i. If we only know the spectrum of a_i we lack sufficient information to compute this as an explicit element of $\mathcal{B}$.

Example 3.15. Suppose a and b are free with respect to some state φ. For short monomials, e.g. ab or ab^2a, free variables behave similar to independent ones

$$\varphi(ab) = \varphi(a)\varphi(b),$$
$$\varphi(ab^2a) = \varphi(a^2)\varphi(b^2).$$

For longer monomials, e.g.

$$\varphi(abab) = \varphi(a^2)\varphi(b)^2 + \varphi(a)^2\varphi(b^2) - \varphi(a)^2\varphi(b)^2.$$

This last expression is representative of the difference between free and independent random variables. For independent random variables, the last two expressions, ab^2a and $abab$, have the same expectation value whereas for free random variables, the expectation values can be as different as 0 and ∞.

Notice also that commutativity precludes freeness, two commuting operators can never be free and vice versa two operators which are free cannot be commuting operators. This of course does not hold for the $\mathbb{1}$-operator, which is free from any other operator in any probability space.

-

Most of the time, we will be working with a select set of free random variables without reference to the free algebras to which they belong. In such a case, an alternative, but equivalent, characterization can be more convenient.

Lemma 3.16. *Let $\big(\mathcal{A}, \mathbb{E}\big)$ be a probability space over $\mathcal{B}$ and $I \subset \mathbb{N}$ a countable index set. IF a set $(X_i)_{i\in I}$ is* free with amalgamation over $\mathcal{B}$*, then*

$$\forall\, n \in \mathbb{N},\, \forall\, p_i \in \mathcal{B}\langle X\rangle \;\; \textit{and} \;\; i(k) \neq i(k+1), \qquad 1 \leq k \leq n,$$

$$\nu_{(a_{i(1)},\ldots,a_{i(n)})}\big(p_1(X_{i(1)}) \cdots p_n(X_{i(n)})\big) = 0$$

if $\forall\, j \in I$,

$$\nu_{a_{i(j)}}\big(p_j(X_{i(j)})\big) = 0.$$

-

Example 3.17 (Fock space picture)**.** For any Hilbert space $\mathcal{H}$, we can define (full) Fock space

$$\mathcal{F}(\mathcal{H}) := \bigoplus_{n\geq 0}^{\infty} \mathcal{H}^{\otimes n},$$

where $\mathcal{H}^0 := \mathbb{C}\Omega$ and for any $h \in \mathcal{H}$ we can define the (left) creation operator $\ell^*(h)$,

$$\ell^*(h)\,\psi := \begin{cases} h & \text{if} \quad \psi = \Omega, \\ h \otimes \psi & \text{if} \quad \langle \psi\,, \Omega\rangle = 0. \end{cases}$$

Its adjoint, $\ell(h)$, acts as an annihilation operator on Fock space,

$$\ell(h)\,\psi_1 \otimes \psi_2 \otimes \cdots \otimes \psi_n = \langle h, \psi_1\rangle\, \psi_2 \otimes \cdots \otimes \psi_n,$$

and kills the vacuum,

$$\ell(h)\,\Omega = 0.$$

In lieu of the more traditional commutation relations, we find

$$\ell(h)\ell^*(h) = \langle h, h\rangle\, \mathbb{1}.$$

Fock space, with it associated vacuum state $|\Omega\rangle\langle\Omega|$, is literally full of operators which are free: *Let h_1, $h_2 \in \mathcal{H}$, the algebras $\mathcal{L}_1$ and $\mathcal{L}_2$ generated by respectively $\{\ell^*(h_1), \ell(h_1\}$ and $\{\ell^*(h_2), \ell(h_2\}$ are free with respect to the vacuum state iff $\langle h_1, h_2\rangle = 0$.*

Assume $\langle h_1, h_2\rangle = 0$, then $\ell(h_1)\ell^*(h_2) = \ell(h_2)\ell^*(h_1) = 0$. To check for freeness, it is sufficient to only look at monomials of the creation and annihilation operators, since any polynomial of creation and annihilation operators of a single vector can be rewritten as a linear combination of monomials in those same creation and annihilation operators. Suppose for instance that

$$p\left(\ell(h), \ell^*(h)\right) = \sum_V c_V\, \ell^{\#(v_1)}(h) \cdots \ell^{\#(v_n)}(h),$$

where V is any series containing only 0's and 1's, $\#(0) = 1$ and $\#(0) = *$. Suppose furthermore that $\langle\Omega|p\left(\ell(h), \ell^*(h)\right)|\Omega\rangle = 0$, then

$$\begin{aligned} &p\left(\ell(h), \ell^*(h)\right) \\ &= p\left(\ell(h), \ell^*(h)\right) - \langle\Omega|p\left(\ell(h), \ell^*(h)\right)|\Omega\rangle \\ &= \sum_V c_V \left[\ell^{\#(v_1)}(h) \cdots \ell^{\#(v_n)}(h) - \langle\Omega|\ell^{\#(v_1)}(h) \cdots \ell^{\#(v_n)}(h)|\Omega\rangle\right], \end{aligned}$$

which is a linear combination of monomials in $\ell(h)$ and $\ell^*(h)$ which all have a zero expectation value under the vacuum state.

Any monomial in creation and annihilation operators of only a single vector h can be further reduced to a canonical form,

$$\ell^*(h)^n \ell(h)^m, \quad n + m > 0, \tag{3.9}$$

since any monomial in $\{\ell^*(h), \ell(h)\}$ has zero expectation value unless it reduces to a multiple of the identity and any long sequence of creation and annihilation operators can be reduced in length with the relation

$$\ell(h)\ell^*(h) = \|h\|^2 \mathbb{1}.$$

It is easy to see that the expectation value of a product of monomials as in (3.9) is always zero.

The reverse implication is immediate. If $\{\ell^*(h_1), \ell(h_1\}$ and $\{\ell^*(h_2), \ell(h_2\}$ *are* free, then $\langle h_1, h_2\rangle = \langle\Omega, \ell(h_1)\ell^*(h_2)\Omega\rangle = 0$.

-

3.3 A combinatorial view on free random variables

In light of chapter 4, it is most convenient to introduce the free convolution using its combinatorial description. This side of free probability was discovered by Speicher [41] and is a highly effective tool for algebraic calculations.

3.3.1 Non-crossing partitions

The combinatorics of free probability are heavily tied to the concept of non-crossing partitions. Non-crossing partitions fulfill a similar role to pair partitions in quantum field theory. In effect, they label the analogues of Feynman diagrams between interacting random variables.

Definition 3.18. 1. Let S be a linearly ordered set. Then $\pi = \{W_1, \ldots, V_p\}$ is a *partition* of S if the $V_i \neq \emptyset$ are disjoint and $\cup_i V_i = S$.

2. The partition π is called *non-crossing* if for all $i, j = 1, \ldots, p$ with $V_i = \{v_1, \ldots, v_n\}$ $(v_1 < \cdots < v_n)$ and $V_j = \{w_1, \ldots, w_m\}$ $(w_1 < \cdots < w_m)$ we have

$$w_k < v_1 < w_{k+1} \iff w_k < v_n < w_{k+1}, \qquad (k = 1, \ldots, m-1). \tag{3.10}$$

3. The V_i are called *blocks* (or *bridges*) of the partition π.

4. If $V_i = \{v_1, \ldots, v_n\}$ is linearly ordered, we denote this by $(v_1, \ldots, v_n)$.

-

It suffices to study the non-crossing partitions of $\mathbb{N}$ or more to the point $(1, \ldots, n)$, $n \in \mathbb{N}$. For any other countable linearly ordered set S, we can always find a map $s : \mathbb{N} \to S$ which preserves the linear order so that non-crossing partitions of $\mathbb{N}$ are mapped to non-crossing partitions of S.

Example 3.19. Consider the linearly ordered set $(1, 2, 3)$. Its partitions are

$$\pi_1 = \big\{\{1\}, \{2\}, \{3\}\big\}, \qquad \pi_2 = \big\{\{1, 2\}, \{3\}\big\}, \qquad \pi_3 = \big\{\{1\}, \{2, 3\}\big\},$$
$$\pi_4 = \big\{\{1, 3\}, \{2\}\big\}, \qquad \pi_5 = \big\{\{1, 2, 3\}\big\}.$$

All of these partitions are non-crossing.

-

Example 3.20. The set $(1, 2, 3, 4)$ is the smallest set where crossing partitions appear. $\pi_1 = \big\{\{1, 3\}, \{2, 4\}\big\}$ is crossing, but $\pi_2 = \big\{\{1, 4\}, \{2, 3\}\big\}$ is not.

-

Catalan numbers

The number of non-crossing partitions of a given set are counted by the so-called Catalan numbers C_n, so named in honor of the Belgian mathematician Eugène Charles Catalan (1814-1894). Any linearly ordered set S with n elements, has C_n non-crossing partitions,

$$C_n = \frac{1}{n+1}\binom{2n}{n} = \frac{(2n)!}{(n+1)!\, n!}.$$

A nice way to summarize this, is by looking at the generating function for the Catalan numbers $c(x)$,

$$c(x) = \frac{1 - \sqrt{1 - 4x}}{2x}.$$

The coefficients of subsequent powers of x in a power series expansion at $x = 0$ are exactly the Catalan numbers.

Drawing partitions

For large sets S, checking whether a given partition is non-crossing can be quite tedious. A graphic depiction of the partition makes it easy to distinguish between crossing and non-crossing partitions. We order the elements of the set S from left to right and put a vertical line under each element. If two (or more) elements belong to the same set, we connect these vertical lines by a horizontal one. We call this a *bridge*, and by analogy, we call the vertical lines *pylons*. E.g. for the partitions $\pi_1 = \big\{\{1,4,5,6\},\{2,3\}\big\}$ and $\pi_2 = \big\{\{1,3,5,6\},\{2,4\}\big\}$ of the set $S = (1,2,3,4,5,6)$,

$$\pi_1 = \big\{\{1,4,5,6\},\{2,3\}\big\} \rightarrow \underline{1\,2\,3\,4\,5\,6},$$

$$\pi_2 = \big\{\{1,3,5,6\},\{2,4\}\big\} \rightarrow \underline{1\,2\,3\,4\,5\,6}.$$

In the second graphic depiction, the bridge connecting the elements of the first block and the bridge connecting the elements of the second block of π_2 cross each other, hence the name *crossing partition*. In the first, the bridge connecting the first and the bridge connecting the second second block of π_1 do not cross, so this amounts to a non-crossing partition.

Sometimes, it is more convenient to represent partitions in the circle. This representation is equivalent to a representation on a line, where the last point is identified with the first to create a circle.

A partial ordering

As a last point, we define a partial order on $NC(n)$. For two partition π_1 and π_2 we say that $\pi_1 \leq \pi_2$ iff each block of π_1 is contained as a whole in one block of π_2. The maximal element of $NC(n)$ is denoted $\mathbb{1}_n$. As a partition, it contains a single block, which connects all the elements of $NC(n)$.

This partial ordering can also be used to construct larger partitions out of several smaller ones. Suppose for instance that π_1 is a non-crossing partition of $NC(n_1)$ and π_2 is a non-crossing partition of $NC(n_2)$. Then we can construct a non-crossing partition of $NC(n_1 + n_2)$ by inserting the partition π_2 between the q^{th} and $(q+1)^{th}$ elements of $\{1,\ldots,q,q+1,\ldots,n_1\}$. This is denoted by $\mathrm{ins}(q, \pi_2 \rightarrow \pi_1)$.

If π_1 is a non-crossing partition of $NC(n_1)$ and π_2 a non-crossing partition of $NC(n_2)$, then we mean by $\pi_1 \cup \pi_2$ the non-crossing partition of $NC(n_1+n_2)$ constructed by adding the blocks of π_1 as a partition of $NC([1,n_1])$ to the set of blocks of π_2 considered as a partition of $NC(n_1+1, n_1+n_2)$.

In calculations where summations over partitions $\{\pi \,|\, \pi \leq \sigma\}$, where σ is a given partition, are involved, the following recursive characterization of non-crossing partitions can be useful.

Lemma 3.21. *A partition $\pi = \{W_1, \ldots, V_n\} \in NC(S)$ is non-crossing if at least one V_i is an interval in S and $\pi \backslash \{V_i\}$ is a non-crossing partition of $S \backslash V_i$.*

Example 3.22. Let S be the linearly ordered set $(1,2,3,4,5,6,7,8)$ and π the partition $\{(1,2,5,8),(3,4),(7)\}$. Both $W_1 = (3,4)$ and $W_2 = (7)$ are intervals of S. $S \backslash (W_1 \cup W_2)$ is the linearly ordered set $(1,2,5,8)$. The remaining block of π is an interval of this reduced set and so π is a non-crossing partition of S.

-

3.3.2 Free cumulants

The free cumulants play a similar role to normal cumulants in regular probability theory. The operator-valued aspect of free probability does however require a more abstract framework to define free cumulants.

Let us first define an object complementary to the distribution of a random variable, the *moments map*.

Definition 3.23 (moments map)**.** Let $(\mathcal{A}, \mathbb{E})$ be a probability space over $\mathcal{B}$. The moments map μ

$$\mu : \bigcup_n \mathcal{A}^n \to \mathcal{B},$$

is given by

$$\mu(a_1, a_2, \ldots, a_n) := \mathbb{E}\left[a_1 a_2 \cdots a_n\right], \qquad a_i \in (\mathcal{A}, \mathbb{E}).$$

The reason that μ is called the moments map is that for (free) random variables a_i

$$\mu(b_0 a_1 b_1, a_2 b_2, \ldots, a_n b_n) = \mathbb{E}\left[b_0 a_1 b_1 \cdots a_n b_n\right],$$

which are the moments of the variables $(a_i)_i$ collected in the distribution of the set $\{a_i\}_i$. The moments map μ thus encodes all the information contained in the distribution of *any* set $\{a_i\}_i \in \mathcal{A}$.

We can go one step further and define a map M

$$M : \bigcup_n \big(NC(n) \times \mathcal{A}^n\big)$$

recursively by

$$M_{\mathbb{1}_n}(a_1,\ldots,a_n) := \mu(a_1,\ldots,a_n), \tag{3.11}$$

$$M_{\pi\cup\sigma}(a_1,\ldots,a_n) := M_\pi(a_1,\ldots,a_k)M_\sigma(a_{k+1},\ldots,a_n), \tag{3.12}$$

$$M_{\mathrm{ins}(p,\sigma\to\pi)}(a_1,\ldots,a_n) := M_\pi(a_1,\ldots,a_pM_\sigma(a_{p+1},\ldots,a_{p+q}),a_{p+q+1},\ldots,a_n), \tag{3.13}$$

where $\sigma\cup\pi$ is the disjoint union of σ and π and $\mathrm{ins}(p,\sigma\to\pi)$ inserts the partition $\sigma\in NC(q)$ after the p^{th} element in S where $\pi\in NC(S)$. A map which satisfies (3.12)-(3.13) is called a *multiplicative map*.

Definition 3.24 (cumulants map)**.** We define the multiplicative map κ through the recursive relation

$$\mu(a_1,\ldots,a_n) = \sum_{\pi\in NC(n)} \kappa_\pi(a_1,\ldots,a_n). \tag{3.14}$$

This map is called the *cumulants map* and the $\kappa_{\mathbb{1}_s}(a_{j(1)},\ldots,a_{j(s)})$ are called the *cumulants* of $\{a_1,\ldots,a_s\}$. We will often denote the cumulants $k_{\mathbb{1}_s}$ as k_s for readability reasons.

In the previous section, we have seen how a non-crossing partition π can be decomposed by subsequent removals of intervals from π. Combined with the multiplicative nature of the function κ, this means that for any π, $\kappa_\pi(a_1,\ldots,a_n)$ can be written as a nested application of the functions $\kappa_{\mathbb{1}_n}$ where n is some natural number. For instance, for the partition $\pi = \big\{\{1,2,5\},\{3,4\}\big\}$, we get

$$\kappa_\pi(a_1,a_2,a_3,a_4,a_5) = \kappa_{\mathbb{1}_3}\big(a_1,a_2\kappa_{\mathbb{1}_2}(a_3,a_4),a_5\big).$$

Since $\mathbb{1}_n$ is the unique element in $NC(n)$ with a block of length n, $\kappa_{\mathbb{1}_n}$ appears exactly once in the summation in (3.14). All other terms are of lower order. The $\kappa_{\mathbb{1}_s}$ are thus uniquely defined through equation (3.14).

Definition 3.25 (mixed cumulants)**.** Consider a probability space $(\mathcal{A},\mathbb{E})$ with free subalgebras $\mathcal{A}_i$. The cumulants

$$\kappa_{\mathbb{1}_s}(a_1,\ldots,a_s)$$

are called *mixed cumulants* if for some $j,k\in\{1,\ldots,s\}$, $a_j\in\mathcal{A}_{q(j)}$, $a_k\in\mathcal{A}_{q(k)}$ and $q(j)\neq q(k)$.

Lemma 3.26. *Consider a probability space $(\mathcal{A},\mathbb{E})$ with free subalgebra's $\mathcal{A}_i$. The mixed cumulants of elements $a_i\in\mathcal{A}_i$ are zero.*

Proof. A proof can be found in [41].

□

Remark 3.27. Lemma 3.26 is often used as an alternative definition of free random variables. Two random variables are then said to be free if their mixed cumulants vanish. If, in applications, freeness is an assumption, this is often a much nicer definition, since it allows direct calculations using cumulants.

Example 3.28. Let us for a moment return to the setting of example 3.15 and calculate some cumulants of the free random variables a and b. Using (3.14), we calculate

$$\begin{aligned}\kappa_1(a) &= \varphi(a),\\ \kappa_1(b) &= \varphi(b),\end{aligned}$$

$$\begin{aligned}\varphi(ab)(=\varphi(a)\varphi(b)) &= \sum_{\pi\in NC(2)} \kappa_\pi(a,b) = \kappa_{\mathbb{1}_2}(a,b) + \varphi(a)\varphi(b),\\ \varphi(a^2) &= \kappa_{\mathbb{1}_2}(a,a) + \varphi(a)^2,\end{aligned}$$

So, $\kappa_{\mathbb{1}_2}(a,b) = 0$ as promised by lemma 3.26 and $\kappa_{\mathbb{1}_2}(a,a) = \varphi(a^2) - \varphi(a)^2$, similar to classical cumulants. By similarity with classical cumulants, k_2 is also called the variance of the probability measure of a.

3.4 Free convolution

In section 3.1.3 we explained how an operator-valued probability measure μ_a can be associated to a general element a from a probability space. In classical probability theory, the convolution describes the probability measure of the sum of two independent random variables. Likewise, the free convolution describes the (operator-valued) probability measure of the sum of two free random variables.

Definition 3.29. Let a and b be two free random variables in some probability space $(\mathcal{A},\mathbb{E})$. The *free convolution* $\mu_a \boxplus \mu_b$ of the probability measures μ_a and μ_b is defined as the probability measure μ_{a+b} of the sum $(a+b)$.

This free convolution can be calculated by turning to cumulants. Since mixed cumulants of free random variables vanish, the cumulants of the sum of free random variables a and b are simply the sum of the cumulants of a and b. All that is required then, is some way of inverting the relation (3.14) between moments and cumulants.

Definition 3.30. Consider a probability space $(\mathcal{A},\mathbb{E})$ over $\mathcal{B}$. The *moment series* G_a of $a \in (\mathcal{A},\mathbb{E})$ is defined as the formal series

$$G_a(b) := \sum_{n=0}^{\infty} \mathbb{E}\left[b(ab)^n\right], \qquad \forall b \in \mathcal{B}. \tag{3.15}$$

Remark 3.31. If $b = 1/z \in \mathbb{C}$, then (3.15) converges for large enough $|z|$ to an analytic function. This function has a unique analytic extension on $\mathbb{C}\backslash\sigma(a)$ which goes to $1/z$ as $z \to \infty$,

$$\mathbb{E}\left[\frac{1}{z-a}\right],$$

which is called the Cauchy (or Stieltjes) transform of the probability measure μ_a. From the Cauchy transform, the original probability measure μ_a can be recovered via a limit procedure,

$$\mu_a = w^*\text{-}\lim_{y\to+0} -\frac{1}{\pi}\operatorname{Im} G_a\left(\frac{1}{x+iy}\right). \tag{3.16}$$

-

Definition 3.32. Consider a probability space $(\mathcal{A}, \mathbb{E})$ over $\mathcal{B}$. The *cumulant series* $K_a(b)$ of $a \in (\mathcal{A}, \mathbb{E})$ is defined as the formal series

$$K_a(b) := \sum_{n=1}^{\infty} k_n(a, \underbrace{ba, \ldots, ba}_{(n-1)\text{ times}}).$$

-

Since mixed cumulants of free random variables vanish, the cumulant series of the sum of two free random variables a_1 and a_2 can be easily restated in terms of the individual cumulant series of a_1 and a_2.

Lemma 3.33. *Consider a probability space $(\mathcal{A}, \mathbb{E})$ over $\mathcal{B}$. For any two random variables a_1 and $a_2 \in (\mathcal{A}, \mathbb{E})$,*

$$K_{a_1+a_2}(b) = K_{a_1}(b) + K_{a_2}(b),$$

where equality holds on the level of formal power series.

-

The relation between moments and cumulants can now be succinctly summarized by the following theorem.

Theorem 3.34. *Consider a probability space $(\mathcal{A}, \mathbb{E})$ over $\mathcal{B}$ and $a \in (\mathcal{A}, \mathbb{E})$. The $\forall\, b \in \mathcal{B}$ the relation*

$$b\Big(\mathbb{1} + K_a\big(G_a(b)\big) \cdot G_a(b)\Big) = G_a(b) \tag{3.17}$$

holds on the level of formal power series.

-

Proof. A proof of this theorem can be found in [41]. We will present another proof in chapter 4 for more general theorem(s) which can be adapted easily to this setting.

□

Remark 3.35. Notice that theorem 3.34 holds only on the level of formal power series in general. If b is chosen to be $z \in \mathbb{C}^+$, the validity of theorem 3.34 can be extended to hold on the level of analytic functions in a neighborhood of ∞. In a few select cases, the domain can be further extended to $\mathbb{C}^+$. In these cases, it becomes feasible to calculate the operator-valued probability measure of a sum of two random variables directly using an analogue of equation (3.16).

-

Example 3.36 (semicircle laws)**.** The semicircle laws have arguably the best-behaved cumulant series, namely, for a semicircle law $w_{m,v}$, the corresponding cumulant series $K(z)$ is

$$K(z) = m + \frac{v^2}{4}z.$$

Suppose a and b are free random variables in a probability space $(\mathcal{A}, \varphi)$, such that the distribution of a follows a semicircle law w_{m_a,v_a} and the distribution of b follows a semicircle law w_{m_b,v_b}. Then the cumulant series of $a + b$ is

$$K_{a+b}(z) = K_a(z) + K_b(z) = (m_a + m_b) + \frac{v_a^2 + v_b^2}{4}z.$$

Using theorem 3.34, it can be seen that the distribution of the sum $a + b$ again follows a semicircle distribution.

In general, the sum of n free random variables which are all distributed according to a semicircle law is again a random variable distributed according to a semicircle law. This behavior is rewarded with the term *stable distribution*.

-

Example 3.37 (random projectors)**.** Equipped with theorem 3.34 we can now calculate explicitly the probability measure associated to the sum of two random projectors in a probability space $(\mathcal{B}(\mathcal{H}), \tau)$ as was promised in example 3.13.

The projectors P_1 and P_2 considered in example 3.13 both have a probability measure,

$$\frac{1}{2}\delta(x) + \frac{1}{2}\delta(x-1),$$

associated to them. Although in principle the cumulant series for both projectors can be calculated directly from definition 3.32, it more convenient to use theorem 3.34. As a formal power series, $C(z) := G_{P_1}(1/z)$ has a formal inverse C^* such that,

$$C(C^*(z)) = z = C^*(C(z)).$$

It should be stressed that such an inverse does not need to exist on the level of (analytic) functions. Even still, if we input the formal inverse C^* into equation (3.17) as $b = 1/C^*(w) = G^*_{P_1}(w)$,

$$K_{P_1}(w) = C^*(w) - \frac{1}{w}. \tag{3.18}$$

Since we know the probability measure associated to P_1, we can calculate the moment series G_{P_1} explicitly,

$$C(z) = G_{P_1}(1/z) = \int_{\Sigma(P_i)} \frac{1}{z-t} d\mu(t) = \frac{1}{2}\left(\frac{1}{z} + \frac{1}{z-1}\right) = \frac{2z-1}{2z(z-1)}, \quad \text{if } |z| > 1.$$

There are two solutions to the equation

$$C(z) = \frac{2z-1}{2z(z-1)} = w,$$

when solved for z. Namely,

$$\left\{\left\{z \to \frac{1+w-\sqrt{1+w^2}}{2w}\right\}, \left\{z \to \frac{1+w+\sqrt{1+w^2}}{2w}\right\}\right\} \tag{3.19}$$

If we put these tentative solution into equation (3.18),

$$K_{P_1}(w) \stackrel{?}{=} \frac{-1+w+\sqrt{1+w^2}}{2w},$$
$$K_{P_1}(w) \stackrel{?}{=} -\frac{1-w+\sqrt{1+w^2}}{2w}.$$

Of the two possible solutions, only the first one provides the required behavior in $w = 0$, namely $K_{P_1}(0) = \mathbb{E}[P_1] = 1/2$. So, we conclude that the cumulant series of P_1 in the region where the series converges, can be written as

$$K_{P_1}(w) = \frac{-1+w+\sqrt{1+w^2}}{2w}.$$

A similar analysis for P_2 would of course result in the same cumulant series, since the probability density functions of both projectors are the same. Through lemma 3.33 we then obtain,

$$K_{P_1+P_2} = \frac{-1+w+\sqrt{1+w^2}}{w}.$$

A direct application of theorem 3.34 says,

$$\frac{1}{z}\left(1 + \frac{-1+G_{P_1+P_2}(1/z)\sqrt{1+G_{P_1+P_2}(1/z)^2}}{G_{P_1+P_2}(1/z)}\right) = G_{P_1+P_2}(1/z),$$

which can be worked out as,

$$G_{P_1+P_2}(1/z) \stackrel{?}{=} \frac{1}{\sqrt{-2+z}\sqrt{z}} \quad \text{or,}$$
$$G_{P_1+P_2}(1/z) \stackrel{?}{=} -\frac{1}{\sqrt{-2+z}\sqrt{z}}.$$

Only the first solution has the required $1/z$ behavior as $z \to \infty$, so we finally obtain that the probability density function associated to the sum $P_1 + P_2$ is

$$\rho_{(P_1+P_2)} = \begin{cases} \frac{1}{\sqrt{x}\sqrt{2-x}}, & \text{if } 0 \leq x \leq 2, \\ 0, & \text{otherwise.} \end{cases} \tag{3.20}$$

-

Fock space picture

Example 3.17 can be expanded upon to construct a canonical realisation of (scalar valued) free random variables as operators on full Fock space.

Theorem 3.38. *Let $\ell^*(h)$ be the creation operator on $\mathcal{F}(\mathcal{H})$ of some normalized vector h. If $\sum_{k=1}^{\infty}|c_s| < \infty$, the series*

$$\ell(h) + \sum_{s=1}^{\infty} c_s \left(\ell^*(h)\right)^{s-1}$$

converges to a bounded operator a on full Fock space. The free cumulants k_s of a are the coefficients c_s.

-

Although this setting is inconvenient as a physical setting, it can often be beneficial to transport a problem concerning free random variables to this setting as it translate the rather unintuitive correlation structure of free random variables into explicit commutation relations.

A free central limit theorem

When dealing with independent random variables, the Gaussian distribution almost inevitably comes into play. The reasons for this ubiquity are the central limit theorems which describe the convergence of normalized sums of independent random variables to a Gaussian distribution.

In free probability theory, the role of the Gaussian distributions is subsumed by the semicircle laws and in full correspondence tot the classical theory, a central limit result describes the convergence of normalized sums of free random variables to a semicircle distribution.

Theorem 3.39 (free central limit theorem)**.** *Let $a_1, a_2, \ldots$ be a sequence of free random variables in a probability space $\mathcal{A}, \varphi$ such that $\varphi(a_i) = 0$ and $\varphi(a_i^2) = 1$. Then the sequence $(a_1 + a_2 + \cdots + a_n)/\sqrt{n}$ converges in distribution to the standard semicircle law.*

-

3.5 Random matrix models

The theory of random matrices has a long and distinguished career in physics and many readers will have encountered random matrices at one point or another. Rather than attempt to condense the theory of random matrices into this single section, we will restrict ourselves to pointing out the connection between certain types of random matrix models and free probability.

The space of $n \times n$ matrices, $\mathcal{M}_n(\mathbb{C})$, admits a simple linear functional, the normalized trace $\mathrm{Tr}_n = 1/n$ Tr which transforms $\mathcal{M}_n(\mathbb{C})$ into a natural probability space $(\mathcal{M}_n(\mathbb{C}), \mathrm{Tr}_n)$. Although, in this sense, any complex matrix can be called a 'random matrix', this name is usually reserves for those types of matrices which can be characterized as matrices which have scalar random variables as entries, i.e. there is an underlying probability space (Ω, φ) which is used as a reservoir for matrix elements. So, in this sense, a random matrix X_n is an element of a probability space $(\mathcal{M}_n(\Omega), \tau_n)$ where $\tau_n = \mathrm{Tr}_n \circ \varphi$.

The difference between the two types of 'random matrices' is not mere mathematical nit-picking. The probability spaces $(\mathcal{M}_n(\Omega), \tau_n)$ and $(\mathcal{M}_n(\Omega), \mathrm{Tr}_n)$ carry two very different notions of probability measures. A probability density function of an $X_n \in (\mathcal{M}_n(\Omega), \mathrm{Tr}_n)$ is a density function f on the space Ω, which leads to the notion of distributions on probability measures.

On the other hand, the probability density function of a random matrix $Y_n \in (\mathcal{M}_n(\Omega), \tau_n)$ is a function on $\mathbb{C}$ and thus has no interpretation as a 'distribution on probability measures'.

These two different types of probability spaces are commonly distinguished by referring to the corresponding probability distribution as either the *empirical eigenvalue distribution* if X_n if $X_n \in (\mathcal{M}_n(\Omega), \mathrm{Tr}_n)$, which is always of the form

$$\frac{1}{n}\left(\delta(\lambda_1) + \cdots + \delta(\lambda_n)\right), \quad \lambda_i \in \Omega,$$

or *mean eigenvalue distribution* if X_n if $X_n\,(\mathcal{M}_n(\Omega), \tau_n)$, which is always of the form

$$\frac{1}{n}\varphi\left(\delta(\lambda_1) + \cdots \delta(\lambda_n)\right),$$

If we consider the limit for $n \to \infty$, both types of random matrices obviously have different convergence properties.

Definition 3.40 (Limit distributions)**.** Consider a sequence of random matrices $(X_n)_{n\in\mathbb{N}_0} \in (\mathcal{M}_d(\Omega), \mathrm{Tr}_n \circ \varphi)$. Then we say that the sequence $(X_n)_n$ has the *limit distribution* μ as $n \to \infty$ if μ is a distribution on $\mathbb{C}\langle X\rangle$ and

$$\mu(X^k) = \lim_{n\to\infty} \mathrm{Tr}_n \circ \varphi\left(X_n^k\right), \quad \forall k \in \mathbb{N}.$$

In addition, we say that the sequence $(X_n)_n$ converges to its limit distribution *almost surely* if

$$\mu(X^k) = \lim_{n\to\infty} \mathrm{Tr}_n\left(X_n^k\right), \quad \forall k \in \mathbb{N}.$$

-

We can also define a notion of convergence for multiple random matrices,

Definition 3.41. Let S be a set. For $n \in \mathbb{N}$, let $(X_n(s))_{s\in S}$ be a family of matrices in $\mathcal{M}_n(\Omega)$. Then we say that the familiy $(X_n(s))_{s\in S}$ has the *limit distribution* μ as $n \to \infty$ if μ is a distribution on $\mathbb{C}\langle X_s | s \in S\rangle$ and

$$\mu(X_{s_1}X_{s_2}\cdots X_{s_m}) = \lim_{n\to\infty} \mathrm{Tr}_n \circ \varphi\left(X_n(s_1)\cdots X_n(s_m)\right),$$

if in addition,

$$\mu(X_{s_1}X_{s_2}\cdots X_{s_m}) = \lim_{n\to\infty} \mathrm{Tr}_n\left(X_n(s_1)\cdots X_n(s_m)\right),$$

we say that the family $(X_n)_n$ converges *almost surely* to its limit distribution.

-

Although, no two finite random matrices are free, in the limit $n \to \infty$ it is natural to look for matrix ensembles which admit an approximation of free random variables.

Definition 3.42. Let $(X_n(s))_{s\in S}$ be a family of random matrices as before. Then the family $(X_n(s))_{s\in S}$ is called *asymptotically free almost everywhere* as $n \to \infty$ if $(X_n(s))_{s\in S}$ has the limit distribution μ almost surely, where

$$\mu(X_{s_1}\cdots X_{s_m}) = \lim_{n\to\infty} \mathrm{Tr}_n\left(X_n(s_1)\cdots X_n(s_m)\right) \ a.s.$$

and $\mathbb{C}\langle X_j\rangle$ is a free factor in $\mathbb{C}\langle X_s | s \in S\rangle$.

-

The most well-known class of random matrix ensembles whose elements converge to asymptotically free almost everywhere random variables, are those that belong to the unitarily invariant matrix ensembles. We have already met such matrices in examples 3.13 and 3.37 as the random projectors P and Q.

The general framework follows similar lines. Let $\mathcal{U}(n)$ be the compact group of unitary matrices of size n. This space carries a natural probability measure, the

Haar measure γ_n. A unitary U_n chosen from $\mathcal{U}(n)$ according to this Haar measure is called a random Haar unitary. Once we have a supply of random Haar unitaries, the following theorem allows us to both construct and recognize asymptotically free almost everywhere random matrices.

Theorem 3.43. *For $n \in \mathbb{N}$, let X_n and Y_n be Hermitian random matrices in a probability space $(\mathcal{M}_n(\Omega), \tau_n)$ and let U_n be a random Haar unitary independent of X_n and Y_n. If the the empirical eigenvalue distribution of X_n (Y_n) converges in distribution almost surely to a compactly supported probability measure μ_X (μ_Y), then $(X_n, U_n Y_n U_n^*)$ is asymptotically free almost everywhere and the limiting distribution of $X_n + U_n Y_n U_n^*$ is the free convolution $\mu_X \boxplus \mu_Y$.*

-

Example 3.44 (Gaussian unitary ensemble)**.** The most celebrated random matrix ensembles are without a doubt the so-called gaussian unitary random matrix ensembles (GUE) on $\mathcal{M}_n(\mathbb{C})$. The elements of this ensemble are the standard Hermitian Gaussian matrices $H(n)$ which satisfy $\forall\, i, j \leq n$,

1. $\{\mathrm{Re}H_{ij}(n)\} \cup \{\mathrm{Im}(H_{ij}(n))\}$ is an independent family of Gaussian random variables,
2. $\varphi(H_{ij}(n)) = 0$, $\varphi(H_{ii}(n)^2) = 1/n$ and if $i < j$, $\varphi(\mathrm{Re}(H_{ij}(n))^2) = \varphi(\mathrm{Im}(H_{ij}(n))^2) = 1/2n$.

We mention these ensembles in particular since they form random matrix models for the semicircle distributions, i.e. both their mean and empirical eigenvalue distribution converge to a semicircle law. Furthermore, since they are unitarily invariant, a family of random matrices drawn from the GUE ensembles converges to a free family of semicircles in the sense of definition 3.42.

-

This correspondence between free random variables and unitarily invariant random matrices is strict. For any family of free random variables, there is a corresponding family of unitarily invariant independent random matrices who converge in distribution almost surely to the family of free random variables. Likewise, if the empirical eigenvalue distribution of each member of a family of unitarily invariant random matrices converge in distribution to a compact distribution, then they converge almost everywhere to a free family of random variables.

This does not mean that any other type of random matrix ensemble cannot lead to free random variables. For instance, random matrices drawn from the GOE, gaussian orthogonal ensemble, which requires i.i.d. gaussian distributed real matrix elements, also converge to a free family.

Other examples of ensembles which lead to free families exist in the literature, but the unitarily invariant ones are by far the most commonly used. In light of

chapter 4, even a subset of the unitarily invariant random matrix ensembles can be considered, the so-called *maximal entropy ensembles*. We will leave the reasons behind this restriction for the introductory sections of the next chapter.

3.6 Resolving free convolution

The preceding sections have already introduced a copious amount of mathematics. Unfortunately, in order to support the extensions of free probability theory needed for chapter 4, some more mathematics should be served to the reader as dessert. And by dessert, we mean of course some ready-made appetizers for the calculations in the following chapter.

Traditionally, a course in operator theory places a large emphasis on the construction and representation of continuous functions on operator algebras. The more restricted class of holomorphic[7] functions is rarely treated explicitly, perhaps because the more common holomorphic functions, such as the exponential and polynomial functions are also entire[8] functions. These can easily be defined on an operator algebra through their Taylor series.

There are two main benefits for considering the spectral representation theory for holomorphic functions rather than the more traditional spectral theory for continuous functions. First, by limiting this discussion to holomorphic functions, or more truthfully, by considering entire functions purely as holomorphic functions, the full force of complex analysis can be brought to bear in this chapter. Especially the Cauchy integral theorem will prove very useful in the following. Secondly, the resolvent mapping $z \mapsto (z - x)^{-1}$ of a operator x is holomorphic on $\mathbb{C}\backslash\sigma(x)$. The important role that resolvent mappings (read: moment generating functions) play in free probability theory combined with the powerful machinery of holomorphic functional calculus allows for a more in-depth study of the analytical properties of free convolution in chapter 4.

A third, but minor advantage concerns the algebraic setting. The spectral theory for continuous functions is most naturally phrased in terms of spectral projectors. In the introductory chapter on free probability it was stressed that all results would be centered on C^*-algebras. Most of the C^*-algebras which will be considered in the remainder of this chapter are freely generated by two or more elements. This type of C^*-algebras does not in general contain any spectral projectors, so the C^*-algebra has to be wrapped up into a larger von Neumann algebra which does contain the spectral projectors. Usually, this is just a minor complication, but one which can be avoided by using holomorphic functional calculus.

[7] Holomorphic functions are complex-valued functions which are complex-differentiable in a neighborhood of every point in their domain.

[8] Entire functions are holomorphic functions whose domain is $\mathbb{C}$. As a consequence, the radius of convergence of a Taylor series expansion in any point is infinite. To physicists, they are more commonly known as 'nice' functions.

Definition 3.45. Let a be bounded element of a C^*-algebra $\mathcal{A}$. A complex number z is said to be in the *resolvent set* $\rho(a)$ if $z\mathbb{1} - a$ is a bijection with a bounded inverse. The complement of $\rho(a)$ is called the spectrum of a, denoted $\sigma(a)$. $R_a(z) = (z\mathbb{1} - a)^{-1}$ is called the *resolvent* of a at z. The function $R_a : \mathbb{C} \to \mathcal{A} : z \mapsto R_a(z)$ is called the *resolvent mapping*. Its domain is the open set $\rho(a)$.

Remark 3.46. In some, mostly physics oriented, texts the resolvent of an operator a is alternatively defined as $(a - z\mathbb{1})^{-1}$. When comparing results with the literature, one should pay attention to this conflicting sign convention. Especially since it is often not mentioned which sign convention is used.

In the context of differential equations, the resolvent is also sometimes referred to as a Green's function or propagator.

Remark 3.47. In the following, z will always be a complex number. Whenever a nonsense expression such as $z - a$ is encountered, it should be read as $z\mathbb{1} - a$.

By analogy with the Cauchy integral formula in complex analysis, a holomorphic functional calculus can be defined on a C^*-algebra by the following definition.

Definition 3.48 (holomorphic functional calculus)**.** Let a be a bounded element of a C^*-algebra $\mathcal{A}$ and f a holomorphic function whose domain $\mathcal{D}$ contains $\sigma(a)$. If a set of positively oriented rectifiable Jordan curves Γ exists on $\mathcal{D}$ such that Γ encloses $\sigma(a)$, then we define $f(a)$ as

$$f(a) := \frac{1}{2\pi i} \int_\Gamma f(z) \frac{1}{z - a} dz,$$

where the integral is of Bochner type.

Example 3.49. It may be illuminating to see how definition 3.48 behaves when the C^*-algebra in question is a matrix algebra. Suppose that A is a finite dimensional selfadjoint matrix. Any such matrix can be diagonalized by some unitary matrix U. The matrix A can then be rewritten as $A = U\Lambda U^*$ where Λ is a diagonal matrix containing the eigenvalues of the matrix A. Using the properties of a Bochner integral, the formula in definition 3.48 can be reduced to a more manageable integral,

$$\begin{aligned} f(A) &= \frac{1}{2\pi i} \int_{\sigma(a)} f(z) \frac{1}{z - A} dz = \frac{1}{2\pi i} \int_{\sigma(a)} \frac{f(z)}{z - U\Lambda U^*} dz \\ &= \frac{1}{2\pi i} U \left(\int_{\sigma(a)} \frac{f(z)}{z - \Lambda} dz \right) U^*. \end{aligned}$$

The argument of this last integral is a diagonal matrix with matrix elements $f(z)/(z - \lambda_i)$ where the λ_i are the eigenvalues of the matrix A. The integral is

easily computed by applying the Cauchy integral theorem for every diagonal matrix element so that

$$f(A) = Uf(\Lambda)U^*,$$

where $f(\Lambda)$ can be understood as element-wise application of the function f to the matrix Λ. This is clearly in line with both the polynomial and continuous functional calculus. For other, more general algebras the calculation strategy remains essentially the same;

1. rewrite the operator a in its eigenbasis by unitary rotation over some unitary u,
2. apply the holomorphic function f element-wise to the operator uau^*, i.e. apply the function f to the eigenvalues of a,
3. rotate the result back to the original basis.

By comparing definition 3.48 to the spectral projector form of continuous functional calculus, one might be tempted[9] to interpret a resolvent $(z-a)^{-1}$ as a spectral projector $P_{\{z\}}$. As we explained, spectral projectors are in general not element of the C^*-algebras under consideration, so the connection is a bit more subtle.

Theorem 3.50 (Stone's formula)**.** *Let a be a bounded self-adjoint element of some C^*-algebra $\mathcal{A}$. Then*

$$s\text{-}\lim_{\epsilon\downarrow 0} \frac{1}{2\pi i} \int_s^t \left(\frac{1}{(x-i\epsilon)-a} - \frac{1}{(x+i\epsilon)-a} \right) dx = \frac{1}{2}\left(P_{[s,t]} + P_{(s,t)}\right),$$

where $P_{[s,t]}$ and $P_{(s,t)}$ are the spectral projectors associated to the operator a on the closed interval $[s,t]$, respectively the open interval (s,t).

The strong operator limit 's-lim' appearing in this theorem provides the necessary convergence path to attain elements which lie outside of the more restrictive C^*-algebras, in this case the spectral projectors.

The inclusion of Stone's formula in this chapter is not mere mathematical pedantry, it also allows for an easy connection between the *expected resolvent mapping* of an operator a under some state or conditional expectation and the associated probability measure of a.

Corollary 3.51. *Let a be a bounded self-adjoint element of some C^*-algebra $\mathcal{A}$. Then for any state φ, the probability density function ρ_φ of the associated measure μ_φ can be obtained from the expected resolvent mapping by*

$$\rho_\varphi(x) = w\text{-}\lim_{\epsilon\downarrow 0} \frac{1}{\pi i} \varphi\left(\frac{1}{(x-i\epsilon)-a} - \frac{1}{(x+i\epsilon)-a} \right).$$

[9] This interpretation is very common in statistical mechanics.

For any conditional expectation $\mathbb{E}$, the operator-valued probability density function $\rho_{\mathbb{E}}$ of the associated measure $\mu_{\mathbb{E}}$ can be obtained from the expected resolvent mapping by

$$\rho_{\mathbb{E}}(x) = w\text{-}\lim_{\epsilon \downarrow 0} \frac{1}{\pi i} \mathbb{E}\left[\frac{1}{(x - i\epsilon) - a} - \frac{1}{(x + i\epsilon) - a}\right].$$

Remark 3.52. Notice that the stronge convergence in theorem 3.50 is watered down to weak convergence in corollary 3.51. In a naive application of Stone's formula, the limit would occur before taking the expectation. In corollary 3.51 the order is reversed and as a consequence the strong limit reduces to a weak one. The exact type of limit depends on the nature of the target space of φ or $\mathbb{E}$. The weak limit also means that Dirac δ-functions and other types of generalized functions can appear in the probability density function.

CHAPTER 4

Household interactions in quantum mechanics

> What is here required is a new kind of statistical mechanics, in which we renounce exact knowledge not of the state of the system but of the system itself.
>
> F.J. Dyson [51]

We consider in this chapter a composite system consisting of a tightly controllable quantum system in contact with a large, mostly inaccessible environment. The interaction between the system of interest and the environment is assumed to be composed of large unitarily invariant random matrices. Similarly spirited models have been considered before in [7, 8, 9, 10, 11, 12, 13].

It is our aim to trace out the interaction terms and in doing so obtain reduced states and dynamics of the stable observables. This problem is generally intractable unless we limit our attention to an extreme form of randomness for the coupling observables, namely to the asymptotic regime of suitably scaled high-dimensional random matrices.

In this limit, the randomness of the interaction terms freezes and mixed moments of both the interaction terms and the unperturbed Hamiltonian become deterministic; the unperturbed Hamiltonian and the interaction terms converge asymptotically to a free family of random variables. Alternatively, if sufficient structure is imposed on the nature of the interaction terms, the family can be free with amalgamation over the algebra of system observables.

The emergence of freeness in this model effectively reduces the information needed to describe the time evolution of the system of interest to an understanding of the spectral properties of the interaction terms and of the full operator structure

of the unperturbed Hamiltonian. If we additionally assume that the initial state of the environment is invariant under the unperturbed dynamics, the needed information further reduces to only knowledge of macroscopic properties of the initial environmental state and spectral properties of the unperturbed Hamiltonian and the interaction terms. It then becomes feasible to explicitly calculate the dynamical behavior of observables associated to the system of interest, irrespective of the type of environment.

It should be stressed that no approximations like replacing Hamiltonians by effective Hamiltonians, assuming particular decoupling schemes or assuming the existence of well-separated time scales are involved. Not surprisingly, the equations governing such reduced dynamics are quite complicated, but some simple cases can be analyzed.

Why study such models?

The original motivation for this chapter was simply the promise of adding a model based on free random variables to the very sparse list of known exactly solvable dynamical systems. Although few and far between in nature, exactly solvable models are ubiquitous in physics, both in textbooks and in active research.

Much like sand castles, most exactly solvable models are built to mirror only the main identifying features of their brick and mortar counterparts, and take considerably less effort to construct. With some notable exceptions, such as the Heisenberg description of the hydrogen atom, exactly solvable models do not correspond to actual physical systems. Rather, they provide a conceptually and computationally simple setting to study a particular phenomenon also encountered in more realistic physical systems less amenable to an exact mathematical description.

Some of these 'simple' models, mostly mean-field or Markovian descriptions [52], can be regarded as course-grained descriptions of the underlying physical systems and these models gain some legitimacy as 'physical models'. Others, such as the Toda lattice [53], remain purely mathematical constructs which mimic a single feature[1] of a particular physical system. Such models are mostly used to identify, qualitatively, the mechanism behind a physical phenomenon.

There is perhaps also an historical note to the popularity of exactly solvable models among physicists. Exactly solvable is often taken to mean *solvable without using a computer*. Many of the models taught in (under)graduate physics courses were developed long before the computational power of digital computers became widespread available. Perhaps, equally important, long before physicists trained to use this new tool became widespread available. Even today, the conceptual simplicity and computational advantage of exactly solvable models over more realistic models, allows them to retain their popularity as teaching tools and testing grounds for new ideas.

For these reasons, we initially did not overly concern ourselves with the physical significance of a *free interaction model*. By itself, the promise of describing large

[1] In the case of the Toda lattice, soliton waves in crystals.

quantum systems in the absence of constraining symmetries or approximations warranted an analysis of such a model.

The central mathematical result which motivated us, was the moment-cumulant relation of theorem 3.34. At its core, it implies that that the sum of two amalgamated free random variables a and b is completely characterized by the distribution of a and b. It further promises a straightforward way to explicitly calculate this sum if the cumulant series of a and b are known. In a dynamical model, this holds the promise of describing in detail the reduced dynamics of a system with a known Hamiltonian H_0 undergoing a *free perturbation* V.

During the analysis of this problem however, we noted three things. Firstly, the existing techniques in free probability theory did not suffice to properly analyze such a dynamical model. We were forced to develop both new analytic and numerical techniques which we believe relevant enough to be considered on their own. A large part of this chapter will thus be devoted to the development and analysis of these techniques[2].

The newly developed techniques give rise to a dynamics in terms of some rather complicated contour integrals over a complex hypersphere. The analysis of these contour integrals is quite involved and only numerical results on this can be obtained. Still, these results represent a substantial and fundamental simplification of the original problem. Moreover, the residual toughness of the problem is inherent to the type of systems we hope to describe.

Secondly, the connection to random matrices provides a direct link to a wealth of existing models in quantum physics [7, 8, 54, 11, 12, 9, 13, 55, 56, 57, 10]. These models span a respectable part of the current research into quantum chaos, decoherence, localization phenomena and quantum disordered systems. Although the physical interpretation of these models differs from case to case, random matrices universally enter these models either as the Hamiltonian of some large quantum system or as a perturbation of a Hamiltonian of a large quantum system. As the matrix size tends to infinity, most of the models referenced above tend to one of the free interaction models we will discuss in this chapter. The advantage of considering the thermodynamic limit is that correlation functions simplify greatly, and a detailed and exact description of the dynamical behavior becomes possible. When appropriate, we will discuss some of the (dis)similarities between the results of the cited articles and our results.

Lastly, the connection to random matrices also provides a heuristic justification for our model as a model of 'generic' environment-assisted dynamics in quantum information theory. Although this realization only struck us after the mathematical analysis of our free interactions models was largely finished, it is perhaps a good idea to reverse the arrow of time and start with a physical motivation for these free interaction models. Under this ordering, it is perhaps also better to coin an alternative name for our free interaction models; *minimal information models*.

[2]Although we will develop these tools in the specific context of open quantum systems, the relevant theorems, 4.2 and 4.16, have straightforward extensions to more general settings.

4.1 Minimal information models

'What happens when we put a quantum computer on our kitchen tabletop?' Answering such a question might very well put you in line for the next Nobel price in physics. Though truthfully, more likely for the development of the quantum computer itself, than for answering the question of what happens to such a device in your kitchen; no-one has as of yet been able to construct a practical quantum computer, not even in controlled laboratory settings. Let alone, has one factorizing RSA codes [1] in his kitchen.

But perhaps we do not actually need a functioning quantum computer to study the above question. Of course this makes the question rather less exciting, and answering it certainly less profitable [58].

Computations in a quantum world

The basic building blocks of a quantum computer are always the same; qudits[3] are used to store information and that information is manipulated by performing unitary operations on those qudits [1]. In this, a quantum computer is like any other finite quantum system. The only quantitative differences between a quantum system able to function as a quantum computer and one that is not, are likely the separation between energy levels within the system, i.e. its Bohr spectrum, and how it interacts with its environment.

The downfall of any quantum computer is its inevitable interaction with the surrounding environment. In general, the interaction with an environment causes correlations to leak out of the system into the environment. If this leakage is severe enough, the resulting correlations between a quantum computer and its environment destroy the logical integrity of the calculation. The computer will most likely still output an answer, but there will be a non-zero chance[4] that the answer is wrong.

In order to work in different environments, in a lab as well as on our kitchen tabletop, a quantum computer should be somewhat agnostic to the environment. In particular, the functioning of a quantum computer should not be compromised by microscopic changes in the environment. Only large, macroscopic and thus manageable differences in the environment should influence the usefulness of a quantum computer.

Given how all finite quantum systems look alike, it is perhaps useful to consider a somewhat more general phrasing of the question in the fist paragraph, 'What happens when we put *any* quantum system on our kitchen table top?' It is strongly

[3] As was explained before, a qubit is the quantum mechanical analogue of a bit, a quantum mechanical two-state system. A qudit is a quantum mechanical system with d energy levels.

[4] This is rather the 'glass half full' interpretation. A more truthful statement would be; there is a non-zero probability of obtaining the correct answer. By making adjustments to the quantum computer on a timescale faster than the natural timescale on which correlation leakage occurs, this non-zero probability can in theory [59, 60, 61, 62] be upgraded to a probability close to one . It is therefore imperative to understand on what timescales this leakage occurs.

suspected, and in fact even the phrasing of this question suggests, that the answer should likewise depend on the full microscopic details of the quantum system, but only *macroscopic* properties of the kitchen tabletop, such as the temperature, thermal and electrical conductivity properties, size of the tabletop, ... If this suspicion is true, then the analysis of this question in terms of the microscopic properties of the quantum system in our kitchen should provide an indication of what type of quantum systems, if any, can be used as a basis for a working quantum computer.

Generic macroscopic environments

Macroscopic properties can be roughly classified into two different types. Properties such as the temperature or pressure determine the macroscopic *state* of a specific environment. We will refer to such properties as *state properties*. Other, such as the mean particle composition of a gas or structural composition of a solid, determine a specific *type* of environment. A wooden tabletop can be at the same temperature as a metal cabinet, but both are of course completely different objects. Such properties we call *interaction properties* if they provide information about the interactions in an environment or the interactions of the environment with the system.

Attempting to describe in detail the evolution of a quantum system in contact with *any* microscopic environment characterized only by such macroscopic information is perhaps overly ambitious. In this chapter we will restrict ourselves to an analysis of those microscopic states and interactions which can be thought of as 'typical' or 'generic' given the macroscopic information we posses.

Typical states

In statistical mechanics, the notion of a 'typical' state is a well-established concept, both theoretical and experimental, and more often than not refers to Gibbs states. There are many, many arguments about the nature of statistical systems which all lead to this same notion of typicality. Rather than pick one and risk confusing the reader, we simply take as a given that if we were to examine the state of our environment in detail, we would most likely find that it is a Gibbs state [52, 63] or some state closely resembling a Gibbs state.

Typical interactions

The idea of a typical interaction is much more debatable. Given two systems, there is no (known) dynamical principle which drives the interaction between those two system towards some typical form. The environmental information we have at our disposal restricts the set of possible microscopic environments and interactions, but does not directly finger a most likely candidate.

However, if this restriction exhausts all the information we have about an environment, we might as well pick one uniformly random from that set. If

we assume that typically the information we have about an environment and its interaction does not favor any particular basis, picking an environment or interaction uniformly random amounts to picking a matrix from a unitarily invariant random matrix ensemble. It is one of the great achievements of free probability theory that in the thermodynamic limit such random matrices all behave similarly. The description of the reduced dynamics then no longer depends on the specific choice from the ensemble and represents in some sense the typical behavior of the system.

Since we know so little about typicality of interactions in large quantum systems, it is correspondingly rather hard to justify the assumption of free interactions. However, there does seem to be experimental evidence to support this assumption. Random matrix ensembles have been used to great success in the study of complex and chaotic quantum systems ever since its inception in the 1950's. The correspondence between for instance the energy level distribution in large nuclei and the spectrum of a large GUE matrix is remarkable [64].

This correspondence even extends far beyond the spectra of large nuclei and for over 2 decades it has been a standing conjecture [65] that *any* quantum chaotic (i.e. non-integrable) system can be accurately described by unitarily invariant random matrices. Usually, the observation that a conjecture has been around for decades is not an indication of its validity, but merely an indication of how hard it is to prove or disprove. In this case, there is an enormous amount of experimental data on quantum chaotic systems. Not a single chaotic system seems to defy this conjecture. So, even if it turns out that there are deviant quantum chaotic systems, the large amount of systems that *can* be accurately described by random matrices alone warrants the name of *typical interactions*.

4.1.1 Microscopic reduced description

An exact quantum mechanical description of the dynamics of both the system of interest S and a specific environment E requires complete knowledge of the initial microscopic state of the combined system as well as a full description of the microscopic interactions within the combined system in terms of a Hamiltonian H.

In theory, much less information is needed to only describe how the system of interest S behaves under the joint evolution of the system and its environment E. The problem then of course becomes, how much and what type of information do we need for such a reduced description. We have looked at such problems in chapter 3 and answered them in the context of probability spaces. We even made some small inroads into how such structures appear in quantum mechanics in section 3.1.1.

The goal[5] of this section is to explain how we can translate the setting of a small, controllable quantum system in contact with a largely unknown environment to the language of probability spaces and introduce the necessary notation.

We assume that the quantum system under study is initially prepared in a

[5] A reader familiar which such concepts can easily skip this section.

specific state σ, such that there are no correlations between observables of the system S and the environment E. In such a case, the initial state ω of the combined system can be mathematically written down as,

$$\omega = \sigma \otimes \rho : \mathcal{S} \otimes \mathcal{E} \to \mathbb{C} : X \mapsto \rho \otimes \sigma(X), \quad \forall\, X \in \mathcal{S} \otimes \mathcal{E},$$

where we have introduced the notation $\mathcal{S}$ for the C^*-algebra which contains the microscopic observables of the system S and $\mathcal{E}$ for the C^*-algebra which contains the microscopic observables of the environment E. The notation ρ for the state of the environment is used only as a placeholder, since we have, as of yet, no way to determine or characterize the microscopic state of the environment. The lack of correlations is evident from this form as,

$$\omega(X \otimes Y) = \sigma \otimes \rho(X \otimes Y) = \sigma(X)\, \rho(Y), \quad \forall\, X \in \mathcal{S} \text{ and } Y \in \mathcal{E}.$$

In terms of probability spaces, the observables X and Y from the above expression are independent random variables in the probability space $(\mathcal{S} \otimes \mathcal{E}, \omega)$.

Likewise, in such a laboratory setting we usually have a (theoretical) understanding of the energy levels present in the system S when isolated from external influences. This information is encoded in the system Hamiltonian H_0^S. In isolation, the evolution of the system S can then be described in the Heisenberg picture as,

$$\alpha_t(X) = e^{-itH_0^S}\, X\, e^{itH_0^S}, \quad \forall\, X \in \mathcal{S}.$$

A similar, though unknown, Hamiltonian evolution should also govern the dynamics of the isolated environment E,

$$\beta_t(X) = e^{-itH_0^E}\, X\, e^{itH_0^E}, \quad \forall\, X \in \mathcal{E}.$$

It is customary to write out the full dynamics of the combined system $(S + E)$ in terms of these Hamiltonians H_0^S, H_0^E and some interaction term V between the system S and the environment E,

$$\gamma_t(X) = e^{-it(H_0^S \otimes \mathbb{1}_\mathcal{E} + \mathbb{1}_\mathcal{S} \otimes H_0^E + V)}\, X\, e^{it(H_0^S \otimes \mathbb{1}_\mathcal{E} + \mathbb{1}_\mathcal{S} \otimes H_0^E + V)}, \quad \forall\, X \in \mathcal{S} \otimes \mathcal{E},$$

or with obvious notational meaning,

$$\gamma_t(X) = e^{-it(H_0^S + H_0^E + V)}\, X\, e^{it(H_0^S + H_0^E + V)} = e^{itH}\, X\, e^{-itH}, \quad \forall\, X \in \mathcal{S} \otimes \mathcal{E}.$$

The quantum mechanical framework is also flexible enough to allow for a reduced dynamical description of only observables of the system S. Under certain general conditions, $\mathcal{S} \otimes \mathcal{E}$ has a unique and faithfull reference state $\tau_{\mathcal{S}\otimes\mathcal{E}}$, called the tracial state with the property that

$$\tau_{\mathcal{S}\otimes\mathcal{E}}(XY) = \tau_{\mathcal{S}\otimes\mathcal{E}}(YX), \quad \forall\, X, Y \in \mathcal{S} \otimes \mathcal{E},$$

which morphs the algebra $\mathcal{S} \otimes \mathcal{E}$ into a natural probability space $(\mathcal{S} \otimes \mathcal{E}, \tau_{\mathcal{S}\otimes\mathcal{E}})$.

The state $\tau_{\mathcal{S}\otimes\mathcal{E}}$ can be alternatively written as the joint application of the tracial states $\tau_{\mathcal{S}}$ and $\tau_{\mathcal{E}}$ on the algebra $\mathcal{S}$ and $\mathcal{E}$,

$$\tau_{\mathcal{S}\otimes\mathcal{E}}(X\otimes Y)=\tau_{\mathcal{S}}(X)\tau_{\mathcal{E}}(Y),\quad \forall\, X\in\mathcal{S} \text{ and } Y\in\mathcal{E}.$$

or the sequential application of the conditional expectation $\mathrm{id}\otimes\tau_{\mathcal{E}}$ defined by

$$\mathrm{id}\otimes\tau_{\mathcal{E}}(X\otimes Y):\mathcal{S}\otimes\mathcal{E}\to\mathcal{E}:\tau_{\mathcal{E}}(Y)X,$$

and the state $\tau_{\mathcal{S}}$,

$$\tau_{\mathcal{S}\otimes\mathcal{E}}=\tau_{\mathcal{S}}\circ(\mathrm{id}\otimes\tau_{\mathcal{E}}).$$

Any other state ω on the global algebra $\mathcal{S}\otimes\mathcal{E}$ can be written in terms of this natural reference state as

$$\omega(X)=\tau_{\mathcal{S}\otimes\mathcal{E}}\left(\mathsf{G}X\right),\quad \forall\, X\in\mathcal{S}\otimes\mathcal{E}.$$

where G is a certain non-negative operator[6] in $\mathcal{S}\otimes\mathcal{E}$ such that $\tau_{\mathcal{S}\otimes\mathcal{E}}(\mathsf{G})=1$. Conversely, any operator G which satisfies these requirements induces a state on the global algebra through the above expression.

Likewise, on the algebras $\mathcal{S}$ and $\mathcal{E}$, any state, in particular the initial states mentioned above, can be written in terms of the respective tracial states as

$$\begin{aligned}\sigma(X)&=\tau_{\mathcal{S}}(\mathsf{S}\,X), &&\forall\, X\in\mathcal{S},\\ \rho(Y)&=\tau_{\mathcal{E}}(\mathsf{E}\,Y), &&\forall\, Y\in\mathcal{E},\end{aligned}$$

with similar conditions on S and E.

We can use these tracial states and the associated conditional expectations to write out a reduced dynamics in the Schrödinger picture as,

$$\omega_t(X)=\tau_{\mathcal{S}}\left(\mathrm{id}\otimes\tau_{\mathcal{E}}\left(e^{itH}\,\mathsf{G}\,e^{-itH}\right)\,X\right),\quad \forall X\in\mathcal{S}.$$

On a d-dimensional algebra $\mathcal{S}$, we can properly normalize the operator $\mathsf{S}_t=\mathrm{id}\otimes\tau_{\mathcal{E}}\left(e^{itH}\,\mathsf{G}\,e^{-itH}\right)$ so that we end up with a time-dependent density matrix σ_t on the algebra $\mathcal{S}$,

$$\sigma_t=\frac{1}{d}\,\mathrm{id}\otimes\tau_{\mathcal{E}}\left(e^{itH}\,\mathsf{S}\otimes\mathsf{E}\,e^{-itH}\right),$$

such that for all times t, the expectation value of an observable X from the algebra $\mathcal{S}$ under the joint evolution of the system S and its environment E is

$$\mathrm{Tr}\,\sigma_t\,X.$$

[6]Note that G is not a density matrix in the usual sense. On a d-dimensional algebra, any state ω can be written in terms of a density matrix ρ as

$$\omega(X)=\mathrm{Tr}\,\rho X.$$

The tracial state on such an algebra is the normalized trace functional $\frac{1}{d}\,\mathrm{Tr}$. So, the operator G associated to the state ω through the above expression would be $d\times\rho$ in such case.

σ_t now encodes all the information necessary to describe in full the behavior of the system S under a joint evolution of the system S and an environment E. In terms of probability spaces, σ_t is the conditional expectation of the operator

$$\frac{1}{d}\, e^{itH}\, (\mathsf{S} \otimes \mathsf{E})\, e^{-itH},$$

in the probability space $(\mathcal{S} \otimes \mathcal{E}, \mathrm{id} \otimes \tau_{\mathcal{E}})$. As was explained in chapter 3, this conditional expectation can be calculated from the joint distribution of the observables H, S and E.

Depending on the information available, it is also sometimes useful to consider σ_t as the matrix populated by the expectation values in the probability space $(\mathcal{S} \otimes \mathcal{E}, \tau_{\mathcal{S}\otimes\mathcal{E}})$ of

$$(E_{ji} \otimes \mathbb{1}_{\mathcal{E}})\, e^{itH}\, (\mathsf{S} \otimes \mathsf{E})\, e^{-itH},$$

where the E_{ij} are the canonical basis elements of the d-dimensional algebra $\mathcal{S}$. This is entirely consistent with the above, as $\tau_{\mathcal{S}\otimes\mathcal{E}} = \tau_{\mathcal{S}} \circ (\mathrm{id} \otimes \tau_{\mathcal{E}})$ and hence,

$$\tau_{\mathcal{S}\otimes\mathcal{E}} \left((E_{ji} \otimes \mathbb{1}_{\mathcal{E}})\, e^{itH}\, (\mathsf{S} \otimes \mathsf{E})\, e^{-itH} \right) = \left[\mathrm{id} \otimes \tau_{\mathcal{E}} \left(e^{itH}\, (\mathsf{S} \otimes \mathsf{E})\, e^{-itH} \right) \right]_{ij}.$$

It also means that in both cases we need exactly the same information, only encoded differently as either the operator-valued joint distribution of H, S and E or the scalar-valued joint distribution of H, S, E and the E_{ij}'s.

Strictly speaking, the joint distributions encode more information than we actually need. For instance, to compute the reduced density matrix σ_t, we do not need to know the expectation (value) of $H\mathsf{E}H\mathsf{S}H^2\mathsf{S}$. In practice, it is difficult to separate the necessary from the non-essential information. Even if such separation would be feasible, the amount of information required to properly characterize the reduced dynamics of the system S far exceeds what we usually know about a system and its environment.

Constructing a reduced description

Ideally, we would like to have a description of reduced evolutions which

1. is easy to calculate, i.e. the computational complexity of the task should scale with the size of the system, not with the size of the (hypothetical environment),

2. allows easy access to physically relevant parameters of the environment, such as temperature, pressure, type of particles, density of states, ...,

3. is robust under small perturbations of the environment. Small changes to the environment part of the Hamiltonian should be easy to handle. Ideally, it should be obvious what the influence of a small perturbation would be.

4. is easy to construct. For large system-environment models, the amount of complex parameters that determine a Hamiltonian scales with the square of the model size. If one only has access to macroscopic observables of the environment, it is hard to justify explicit values for all parameters and it is not obvious what the physically relevant parameter ranges are.

With perhaps the exception of being 'easy to calculate', we propose that a model based on free random variables presents exactly such a description. The basic setup of such a model is introduced in the following two sections.

4.1.2 Free interactions in quantum systems

In this section, and the following one, we present two general models based on free random variables. As detailed in chapter 3, a distinction can be made between random variables which are simply free in the natural probability space $(\mathcal{S}\otimes\mathcal{E}, \tau_{\mathcal{S}\otimes\mathcal{E}})$ and random variables which are free with amalgamation over the system algebra $\mathcal{S}$ in the probability space $(\mathcal{S}\otimes\mathcal{E}, \mathrm{id}\otimes\tau_{\mathcal{E}})$. The former type will be explained in this section and the latter in the following section.

To cut back a little on the already heavy notation, below we will use the shorthands τ for $\tau_{\mathcal{S}\otimes\mathcal{E}}$ and $\mathbb{E}$ for $\mathrm{id}\otimes\tau_{\mathcal{E}}$.

States of the global system

As per the general microscopic picture explained in section 4.1.1, we assume that initially the global system starts out in a separable state such that no correlations exist between observables of the system algebra $\mathcal{S}$ and those associated to the environment $\mathcal{E}$. In the probability space $(\mathcal{S}\otimes\mathcal{E}, \tau)$, we can associate to such a state, two positive operators S and E so that the expectation values under the initial state ω can be calculated as

$$\tau\left(\mathsf{S}\otimes\mathsf{E}\,X\right), \quad \forall\, X\in\mathcal{S}\otimes\mathcal{E}.$$

We assume that the operator structure of S is well-known to an observer and E describes a state which is invariant under the dynamics of the environment in isolation. This condition is both likely to be true and necessary to facilitate a numerical solution. If the environment is initially not in a state invariant under the dynamics, the environment will react too violently to the dynamics to be amenable to our model. When the explicit dependence of the state E on the Hamiltonian H_0^E is needed to progress the calculations, we will canonically denote it as $\mathsf{E}(H_0^E)$.

If and when we restrict our attention to only the system S, we can content ourselves with using the density matrix formalism. In such situations, we use the notation $\sigma(t)$ to denote the time-evolved density matrix of the system S in the Schrödinger picture.

Hamiltonian of the global system

We suppose that the Hamiltonian H governing the evolution of the combined system can be written as

$$H = H_0^S + H_0^E + V, \tag{4.1}$$

such that H_0^S is the Hamiltonian of the system S in isolation, H_0^E the Hamiltonian of the environment in isolation and V is a random matrix interaction drawn from a unitarily invariant random matrix ensemble. In the thermodynamic limit, this choice for the interaction V assures that V is free from H_0^S, H_0^E and $\mathsf{S} \otimes \mathsf{E}$ (or $\sigma(0) \otimes \mathsf{E}$).

The assumption of freeness guarantees that we have sufficient information to calculate the reduced dynamics of the system S,

$$\sigma(t) = \mathbb{E}\left[e^{it(H_0+V)}(\sigma(0) \otimes \mathsf{E})e^{-it(H_0+V)} \right]. \tag{4.2}$$

As explained in section 4.1.1 a sufficient, though not necessary, measure for the information needed to calculate reduced evolutions is the joined distribution of H_0, V and $\sigma(0)$ and $\mathsf{E}(H_0^E)$.

The interplay between H_0, $\sigma(0)$ and $\mathsf{E}(H_0^E)$ is determined by the explicit choice for the operator H_0^S and density matrix $\sigma(0)$. Because we have opted to only describe initially uncorrelated states, H_0^E and $\mathsf{E}(H_0^E)$ are independent (in the classical probability sense) from H_0^S and $\sigma(0)$. Furthermore, as suggested by our notation, $\mathsf{E}(H_0^E)$ is simply a function of H_0^E. The joint distribution of all these variables is thus easily constructed.

The interaction between the above observables and V is completely resolved by the assumption of freeness. Any and all correlations between H_0 and V can be calculated from the knowledge of the spectral measures of H_0 and V, as explained in chapter 3.

4.1.3 Amalgamated free interactions in quantum systems

An alternative point of view, is to study the global system in the probability space $(\mathcal{S} \otimes \mathcal{E}, \mathbb{E})$. The considerations on the initial state and Hamiltonians H_0^S and H_0^E can simply be copied over from the previous section. Only the nature of the interaction changes from the the previous case to this setting.

The obvious modification to the conditions on the interaction V is to now restrict it to a random variable free from the operators H_0 and $\mathsf{S} \otimes \mathsf{E}$ with amalgamation over the system algebra $\mathcal{S}$. However, this does not provide enough information to calculate the dynamical behavior of the reduced density matrix. At the end of section 4.1.1 is was pointed out that a sufficient amount of information is encoded in the joint distribution of the above operators. In particular, the assumption that V is free from H_0^S with amalgamation over $\mathcal{S}$ by itself does not provide any information on how $\mathbb{E}[V]$ behaves as an operator on the algebra $\mathcal{S}$.

Although amalgamated free random variables allow us to study more general types of interactions, the price we have to pay is that we have to provide more information on the type of interaction. For this class of models we will always assume that the interaction V is of the form,

$$V = \sum_{i,j} E_{ij} \otimes V_{ij}, \tag{4.3}$$

such that the operators V_{ij} form a free family of Hermitian operators in the probability space $(\mathcal{E}, \tau_{\mathcal{E}})$. Additionally, we also assume that this family is free from the environment Hamiltonian H_0^E in the same probability space. It can easily be seen that such a V is indeed free with amalgamation over $\mathcal{S}$ from the other relevant operator parameters in our model.

Although, in principle, the explicit form (4.3) of the interaction V provides sufficient information to calculate the reduced dynamics, the resulting equations are too complex to handle.

It is also possible to generalize this construction slightly by removing the assumption[7] that *all* V_{ij} are free. The price for dropping such an assumption is always that explicit correlation functions have to be specified, either by providing them directly or describing the commutation relations between the new V_{ij}. We will not handle such generalizations explicitly.

4.2 An (amalgamated) free toy model

The models introduced in the previous section cover quite a lot of ground and are perhaps still too general to model specific systems. The only aspects of these models that are set is stone, are (i) the assumption of freeness for the interaction term(s); and perhaps, given our presentation in chapter 3, (ii) the boundedness of the global Hamiltonian. Of the two, only the assumption of freeness is an actual restriction. The boundedness of the global Hamiltonian can be thrown overboard if so desired. Of course, this results in some quite nasty mathematical problems which always seem to accompany such carelessness about bounds.

With or without the restriction of a bounded global Hamiltonian, the physical situations we hope to describe with the models in section 4.1 range from 'a qubit freely interacting with a random electromagnetic field' to 'a quantum computer freely interacting with our kitchen tabletop'. Both situations, and every situation in between, are handled by essentially the same general set of equations in our models. We will introduce these equations shortly.

On the one hand, such scale-invariance is a rather impressive feature of our models and one that is rarely encountered in other models. On the other hand, the physical behavior of a qubit freely interacting with a random electromagnetic field

[7] For instance, in [46, 47] some aspects of such a model were analyzed in the situation where some V_{ij} were not free, but identical.

is, or rather, is expected to be somewhat different from the behavior of a quantum computer on our kitchen tabletop. Our models have enough wiggle room to allow for such different behavior, but as a consequence the analysis of our models and the subsequent equations depends very much on the explicit choices made for the parameters in our models.

It is therefore rather difficult to summarize exactly how arbitrary systems react to the assumption of freeness. The behavior depends very much on the undetermined parameters in our models; (i) the Bohr spectrum of the Hamiltonian H_0^S, (ii) the distribution of the unperturbed Hamiltonian H_0^E, (iii) the distribution of the interaction V, and (iv) the initial state of the global system.

It is however still rather enlightening to see how our equations behave in specific situations. So, for both of the models introduced in section 4.1 we will discuss a single example which showcases the effect of freeness in a simple, but hopefully representative setting.

Although we call this explicit example a 'toy model', we only use this term to separate it from the more general models described in the previous section. In contrast to what is typically considered a toy model, our model, or more truthfully, the random matrix version of our model, has been used to describe actual physical systems with rather good results. A recent comparison between experiment and model is described in [55].

4.2.1 A model system

Hamiltonian of the system S The system S in our canonical example is the simplest possible quantum system; a qubit. The single identifying feature of such a system is the energy gap between the two eigenstates of the Hamiltonian H_0^S. It will be convenient to write out the Hamiltonian H_0^S as

$$H_0^S = -\epsilon\,|0\rangle\langle 0| + \epsilon\,|1\rangle\langle 1|,$$

so that the energy gap is precisely $2\,\epsilon$. We will refer to the basis $\{|0\rangle, |1\rangle\}$ as the *computational basis* of the system S.

Our general equations scale rather well to systems with more than one qubit, or even to the more general case of a qudit; a multi-level system with arbitrary energy levels. The one qubit case suffices though to showcase the necessary steps in an analysis of a system with free interactions.

Initial state of the system S In all cases, we assume that initially the system S can be put in an arbitrary state by the hypothetical experimentator, but we do not allow for initial entanglement between the system and its environment. In the following, we use the notation $\sigma(0)$ as a placeholder for this state's density matrix.

4.2.2 A model environment

Hamiltonian of the environment E The environment of our canonical example is assumed to be described by a Hamiltonian H_0^E characterized by a finite, uniform energy spectrum, i.e. the probability density function $\mu_{H_0^E}$ is of the form

$$\mu_{H_0^E}(x) = \begin{cases} \frac{1}{2h} & \text{if } -h \leq x \leq h, \\ 0 & \text{otherwise.} \end{cases}$$

where h is some finite, positive number.

The spectrum of H_0^E is purposely rather bland. In this way, any effects on the system S arise because of the free nature of the coupling and not from the internal structure of the environment. The parameter h controls the norm of the Hamiltonian H_0^E so that both wide and narrow spectral environments can be studied.

The probability distribution averages to zero for practical purposes, but also since any offset is not physically relevant. An offset can easily be implemented by the transformation $H_0^E \to H_0^E + \lambda \mathbb{1}$. Such a transformation does not influence the qualitative dynamical behavior of the global system. The only result such a transformation produces, is an overal phase shift in the state of the environment.

The explicit choice of the above H_0^E does not in any way trivialize the analysis of the model. More complicated spectra can be (and have been) analyzed in an identical manner.

Initial state of the environment E To combat any effects arising because of (thermal) equilibration in the environment, we assume that initially the environment E is in a state invariant under the dynamics induced by H_0^E. In particular, such a state can be a thermal state or an eigenstate of the Hamiltonian H_0^E.

This assumption also reduces the numerics of the problem considerably and allows us to restrict the description of H_0^E to its probability density function. To treat more general initial environmental states, the full operator structure of the density matrix of the state and the Hamiltonian H_0^E should be specified. The provision of such detailed information about the environment takes us well outside of the philosophical framework of our models and as such will not be considered here.

4.2.3 A model interaction

A model free interaction The distribution of the interaction term(s) in our examples is assumed to follow a semicircle law. For the free interaction model this means that the interaction term V has a probability density function (under the

state τ) of the form

$$\mu_V(x) = \begin{cases} \frac{2}{\pi v^2}\sqrt{v^2-(x-m)^2} & \text{if } -m-v \leq x \leq m+v, \\ \\ 0 & \text{otherwise.} \end{cases}$$

The parameter m controls the mean expectation of the interaction and $v > 0$ the variance of the interaction. More physically, it turns out that the variance squared v^2 is akin to the interaction strength in this model.

Without loss of generality, we can assume that the mean m is zero. Any non-zero mean has the net effect of lifting the energy levels ϵ and $-\epsilon$ in the system by the same amount m and so has no net physical effect on the global dynamics.

A model amalgamated free interaction Likewise, in the more complicated case of the amalgamated free model, the b_{ij} are assumed to form a free family of semicircle laws, each with their own mean m_{ij} and variance v_{ij}. In the qubit version of our toy model, the interaction V can thus be written as (an element of $\mathcal{M}_d(\mathcal{E})$),

$$V = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22}. \end{pmatrix}$$

where $b_{12} = b_{21}^*$ so that V is Hermitian. Since we have opted[8] to only consider Hermitian random variables, this is equivalent to $b_{12} = b_{21}$.

Why semicircles?

- The semicircle laws are without a doubt the most celebrated and most frequently used distributions in free probability theory. As was explained in example 3.44, these distributions enter our model most naturally as limits of random GUE matrix interactions.

- Alternatively, they can be characterized by a maximum entropy principle [39] under the constraint that the variance of the distribution is equal to some constant v. As indicated above, fixing the variance of the interaction distribution is akin to fixing the strength of the interaction. Applying the maximum entropy principle is then tantamount to characterizing the interaction V only in terms of our knowledge of the interaction strength and discarding all other information. In contrast to for instance a Lindbladian approximation, there are no bounds on the interaction strength; it can be weak or strong.

- This interpretation is strengthened by the fact that effectively the semicirle distribution functions as a first order approximation to any free random

[8] We have not discusses non-Hermitian random variables before. The interested reader can consult any of the references mentioned in chapter 3 for an exposition on this extension.

variable. Similiar to the Gaussian ensemble in classical probability theory, the (free) cumulants of the semicircle laws are all zero except for k_1 and k_2. The cumulant function $K_V(z)$ is thus the very simple (analytic) function

$$K_V(z) = k_1(V) + k_2(V)z = m + v^2 z.$$

If we cut off the cumulant series of *any* random variable after the first order, we effectively approximate it by a suitable semicircular variable.

This is also true if we consider amalgamated free random variables. For the amalgamated free toy model, the $\mathcal{S}$-valued cumulant function is,

$$K_V(\mathbf{X}) = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} + \begin{pmatrix} v_{11}^2 X_{11} + v_{12}^2 X_{22} & v_{12}^2 X_{21} \\ v_{12}^2 X_{12} & v_{12}^2 X_{11} + v_{22}^2 X_{22} \end{pmatrix}.$$

Similar to the plain free case, operator-valued semicircular elements function as a first-order approximation to more general random variables.

- One of the biggest problems in practical applications of free probability theory is that calculating the cumulant series of a general distribution is a rather complicated process. Apart from the basic definition in chapter 3, there is no useful numerical way to calculate this object. The basic definition suffers as a tool since it does not allow for a straightforward way to approximate a cumulant series. If a cumulant series is broken off at some random order of z (or $\mathbf{X}$), the resulting series does not in general correspond to the cumulant series of a distribution. In our model, this leads to non-physical interactions and in some cases, negative probabilities for occupation numbers of energy levels. Unfortunately this means that in terms of cumulant series, the semicircle laws are unique as approximating distributions.

- Another justification for the use of semicircle laws is the central limit theorem for free random variables [39].

  Theorem 4.1 (Free central limit theorem)**.** *Let a_1, a_2, ... be a free sequence of random variables in the probability space $(\mathcal{A}, \tau)$ such that $\tau(a_i) = 0$ and $\tau(a_i^2) = 1$ and all other moments are bounded. Then the sequence $(a_1 + a_2 + \cdots + a_n)/\sqrt{n}$ converges in distribution to the standard semicircle law with a zero average and variance $v = 1$.*

  If the total interaction V can be considered as a sum of interactions between the system and various (overlapping) parts of the environment, then it becomes likely that this free central limit theorem becomes applicable and a semicircle law for the total interaction V becomes appropriate. In particular, this situation is rather likely for systems with a high degree of disorder.

- Lastly, dynamical models using random matrix interactions (e.g. [8, 9]) seem to mostly involve only GUE matrices. As semicircle laws are the thermodynamical limits of such matrices, results obtained for such models can be most easily compared to our results in this toy model.

4.3 Hamiltonian specter of freely interacting systems

The mathematical derivation of the dynamical behavior of this system is quite involved, but can be split up into several more manageable pieces. The first step in this scheme, is a modification of theorem 3.34. By itself, theorem 3.34 does not suffice to calculate an expression such as (4.2). It only provides information about the *spectrum* of the sum $H = H_0 + V$, but discards all information about the operator structure of this sum. In particular, this means only expressions which do not contain any other operators than H can be calculated using theorem 3.34. In (4.2), the appearance of the initial state in the form of the operator $\mathsf{S} \otimes \mathsf{E}$ thus prevents a direct application of this theorem.

4.3.1 A modified moment cumulant relation

The workhorse in the calculations on this model is a rescaled version of the conditionally expected resolvent mapping of the Hamiltonian H onto the system of interest S,

$$\mathbf{r}(z) := \frac{1}{d}\,\mathbb{E}\left[\frac{1}{z-H}\right], \quad \text{where } d = \dim(S), \tag{4.4}$$

which is a holomorphic function on $\mathbb{C}\backslash\Sigma(H)$. It is also convenient to introduce the notation,

$$r(z) := \sum_{k=1}^{d} \mathbf{r}_{kk}(z) = \tau\left[\frac{1}{z-H}\right],$$

again a holomorphic function on $\mathbb{C}\backslash\Sigma(H)$.

The immediate relevance of $\mathbf{r}(z)$ is its relation to the spectral measure of the operator H, which can be calculated from the expected resolvent using Stone's formula (corollary 3.51). Alternatively, if one is only interested in expectations of holomorphic functions of H, there is no need to calculate the spectral measure. Instead, for any f, $\mathbb{E}\left[f(H)\right]$ can be calculated as,

$$\mathbb{E}\left[f(H)\right] = \frac{d}{2\pi i} \oint_{\Sigma(H)} dz\, f(z)\, \mathbf{r}(z).$$

Later on, in section 4.4, we will also show that the reduced density matrix $\sigma(t)$ can be written in terms of complex integrals involving only this rescaled expected resolvent mapping $\mathbf{r}(z)$.

Additionally, the expected resolvent mapping also has its use in studying the restriction of the global equilibrium states to the local system S in section 4.3.4.

The model we are considering in this section is set in the probability space $(\mathcal{S} \otimes \mathcal{E}, \tau)$, not the space $(\mathcal{S} \otimes \mathcal{E}, \mathbb{E})$, which is the natural probability space to consider. In order to exploit the freeness of the interaction, we need to rephrase the

rescaled expected resolvent $\mathbf{r}(z)$ in terms of expectation values under the state τ of operators belonging to $\mathcal{S}\otimes\mathcal{E}$. As a random variable, $\mathbf{r}(z)$ belongs to the probability space $(\mathcal{S},\tau_{\mathcal{S}})$. However, the matrix elements of $\mathbf{r}(z)$ can be written as expectation values of random variables belonging to $(\mathcal{S}\otimes\mathcal{E},\tau)$,

$$\begin{aligned}\mathbf{r}_{ij}(z) &= \frac{1}{d}\,\mathrm{Tr}_{\mathcal{S}}\left(E_{ji}\,\mathbb{E}\left[\frac{1}{z-H}\right]\right) = \frac{1}{d}\,\mathrm{Tr}_{\mathcal{S}}\left(\mathbb{E}\left[(E_{ji}\otimes\mathbb{1}_{\mathcal{E}})\frac{1}{z-H}\right]\right)\\ &= \tau_{\mathcal{S}}\left(\mathbb{E}\left[(E_{ji}\otimes\mathbb{1}_{\mathcal{E}})\frac{1}{z-H}\right]\right) = \tau\left[(E_{ji}\otimes\mathbb{1}_{\mathcal{E}})\ \frac{1}{z-H}\right],\end{aligned}$$

where the E_{ij} are the standard matrix basis elements in the computational basis of the system S, i.e. $E_{ij}=|i\rangle\langle j|$.

Theorem 4.2. *Let H be the Hamiltonian of a dynamical model as proposed in section 4.1.2, so that H can be written as H_0+V, where V is free from H_0 in the probability space $(\mathcal{S}\otimes\mathcal{E},\tau)$. In a neighborhood of ∞, the matrix elements of the renormalized expected resolvent $\mathbf{r}(z)$ are the unique solutions of the self-consistent set of equations,*

$$\mathbf{r}_{ij}(z) = \delta_{i,j}\,\frac{1}{d}\int d\mu_{H_0^E}(\lambda)\,\frac{1}{z-\epsilon_i-\lambda-K_V\left(\sum_k \mathbf{r}_{kk}(z)\right)}, \tag{4.5}$$

where K_V is the cumulant series of the interaction V and $\mu_{H_0^E}$ the spectral measure associated to the environmental part of the non-interacting Hamiltonian H_0. Alternatively, these equations can be written as,

$$\mathbf{r}_{ij}(z) = \frac{1}{d}\left(\mathbb{E}\left[\frac{1}{z-H_0-K_V(\sum_k \mathbf{r}_{kk}(z))}\right]\right)_{ij}.$$

-

Proof. we can rewrite (4.4) in terms of the non-interacting Hamiltonian and the interaction term V.

$$\mathbf{r}_{ij}(z) = \tau\left[(E_{ji}\otimes\mathbb{1}_{\mathcal{E}})\,\frac{1}{z-H_0-V}\right].$$

For sufficiently large $|z|$, the Neumann series,

$$N_{ij}(z) := (E_{ji}\otimes\mathbb{1}_{\mathcal{E}})\sum_{n=0}^{\infty}(z-H_0)^{-1}\left(V(z-H_0)^{-1}\right)^n, \tag{4.6}$$

converges in norm to the matrix elements of the resolvent mapping $R(z)$. Notice that it converges absolutely and we can thus rearrange terms in this series without perturbing the convergence. Equally important, all subseries converge, albeit to a different element in the algebra $\mathcal{S}\otimes\mathcal{E}$.

Existence of solutions

We begin by proving that if the Neumann series converges, it leads to the above equations. We can rewrite the expectation of (4.6) in terms of free cumulants where we use the shorthands $A = (z - H_0)^{-1}$ and $A^{(ij)} = (E_{ji} \otimes \mathbb{1}_{\mathcal{E}})(z - H_0)^{-1}$ to compact the equations slightly,

$$\begin{aligned} n_{ij}(z) := \tau\left[N_{ij}\right] &= \tau\left[A^{(ij)}\right] + \sum_{n=1}^{\infty} \tau\left[A^{(ij)}(VA)^n\right] \\ &= \tau\left[A^{(ij)}\right] \\ &\quad + \sum_{n=1}^{\infty} \sum_{\pi \in NC(2n)} k_\pi(A^{(ij)}, \dot{V}, A, \underbrace{V, A, \ldots, V, A}_{(n-1) \text{ times}}). \end{aligned}$$

We can rearrange[9] the terms in the sum over $NC(2n)$ according to the number of elements connected by the bridge that starts at the dotted V; the first V which appears in the above expansion. Since A and V are free, the only non-zero cumulants are those which correspond to partitions where the bridges connect only A's or only V's or equivalently blocks with only even or only odd numbers.

For any n, there are exactly n V's, so the bridge that contains $\dot{V}$, connects at most n elements. If we denote the bridge which contains $\dot{V}$ by W_1,

$$\begin{aligned} n_{ij}(z) =& \tau\left[A^{(ij)}\right] \\ &+ \sum_{n=1}^{\infty} \sum_{s=1}^{n} \sum_{\substack{W_1, \\ |W_1|=s, \\ 2 \in W_1}} \sum_{\substack{\pi = \{W_1, \ldots\} \\ \pi \in NC(2n+1)}} k_\pi(A^{(ij)}, \dot{V}, A, V, A, \ldots, V, A) \end{aligned} \tag{4.7}$$

If $W_1 = (w_1 = 2, \ldots, w_s)$, then each remaining block W_k in $\pi = \{W_1, \ldots\}$ is wedged between some $w_{j(k)}$ and $w_{j(k)+1}$ on the circle, i.e.

$$\forall\, W_k \in \pi \,\text{and}\, k \neq 1, \exists!\, j(k) \in \{1, \ldots, 2n\} \nrightarrow W_k \subset [w_{j(k)}, w_{j(k)+1}],$$

where $w_{s+1} := w_1$ and $[w_{j(k)}, w_{j(k)+1}]$ denotes an oriented circle segment. In other words, π can be decomposed as the union of s partitions σ_k and the bridge W_1,

$$\pi = \{W_1\} \cup \sigma_1 \cup \cdots \cup \sigma_s,$$

such that for all $k \leq s$, σ_k is a non-crossing partition of $\{w_k{+}1, w_k{+}2, \ldots, w_{k+1}{-}1\}$. As we stated before, the corresponding cumulant k_π, or in this case,

$$k_{\{\{W_1\} \cup \sigma_1 \cup \cdots \cup \sigma_s\}}(A^{(ij)}, \dot{V}, A, \ldots, V, A)$$

[9] This rearrangement does not alter the convergence properties of the Neumann series since we only permute terms under the sum over $NC(2n)$.

is only non-zero if W_1 bridges only V's . For any k, this means that $\mathbb{1}_{[w_k+1,w_{k+1}-1]}$ corresponds to a bridge connecting all elements in the set

$$(\dot{A}, V, A, \ldots, V, \ddot{A}),$$

where $\dot{A}$ is the $(w_k+1)^{th}$ element in the original word and $\ddot{A}$ the $(w_{k+1}-1)^{th}$ element. The partition σ_s is a bit special, as in general the first two elements it connects are $A^{(ij)}$ and some A. The subsequent arguments of k_{σ_s} do follow the same pattern as for the other partitions. If we plug this information into equation (4.7), we get

$$\begin{aligned} n_{ij}(z) = \tau\left[A^{(ij)}\right] + \sum_{n=1}^{\infty}\sum_{s=1}^{n} \sum_{\substack{W_1,\\ |W_1|=s,\\ 2\in W_1}} \sum_{\substack{\pi=\{W_1,\ldots\}\\ \pi\in NC(2n+1)}} \\ k_{W_1}(\dot{V},\ldots,V)k_{\sigma_1}(A,V,A,\ldots,V,A)\cdots k_{\sigma_{s-1}}(A,V,A,\ldots,V,A) \\ \times k_{\sigma_s}(A^{(ij)},A,V,A,\ldots,V,A). \end{aligned}$$

The summation over W_1 is equivalent to a summation over a set $\{w_1,\ldots,w_s\}$ if we demand that $2 = w_1 < \cdots < w_s \leq 2n$. The summation over π can then be replaced by a summation over all σ_k with appropriate conditions. We also rewrite k_{W_1} as k_s to signify that it only depends on W_1 through the number s.

$$\begin{aligned} n_{ij}(z) = \tau\left[(E_{ji}\otimes\mathbb{1}_E)A\right] + \sum_{n=1}^{\infty}\sum_{s=1}^{n} \sum_{\substack{2=w_1<\cdots<w_s\leq 2n\\ w_k \text{ even}}} \sum_{\substack{\sigma_k\in\\ NC([w_k+1,w_{k+1}-1])}} \\ k_s(\dot{V},\ldots,V)k_{\sigma_1}(A,V,A,\ldots,V,A)\cdots k_{\sigma_{s-1}}(A,V,A,\ldots,V,A) \\ \times k_{\sigma_s}(A^{(ij)},A,V,A,\ldots,V,A). \end{aligned}$$

We change variables one last time and write $i_k := (w_{k+1}-w_k-2)/2$ for $k<s$ and

$i_s := (2n - w_s)/2$,

$$
\begin{aligned}
=&\tau\left[A^{(ij)}\right] + \sum_{n=1}^{\infty}\sum_{s=1}^{n} \sum_{\substack{i_1,\dots,i_s\in\\ \{0,\dots,n-1\}\\ i_1+\cdots+i_s=\\ n-s}} \sum_{\sigma_k\in NC(2i_k+1)} \\
&k_s(\dot{V},\dots,V)k_{\sigma_1}(A,V,A,\dots,V,A)\cdots k_{\sigma_{s-1}}(A,V,A,\dots,V,A) \\
&\times k_{\sigma_s}(A^{(ij)},A,V,A,\dots,V,A). \\
=&\tau\left[A^{(ij)}\right] + \sum_{n=1}^{\infty}\sum_{s=1}^{n} \sum_{\substack{i_1,\dots,i_s\in\\ \{0,\dots,n-1\}\\ i_1+\cdots+i_s=\\ n-s}} k_s(\dot{V},\dots,V) \\
&\times \tau\left[A\underbrace{VA\cdots VA}_{i_1 \text{ times}}\right]\cdots\tau\left[A\underbrace{VA\cdots VA}_{i_{s-1} \text{ times}}\right]\tau\left[A^{(ij)},A,\underbrace{VA\cdots VA}_{i_s \text{ times}}\right].
\end{aligned}
$$

In a leap of faith, we now rearrange all the terms in the summation, including terms corresponding to different values of n. We choose one index i_j and hold all other indices, as well as s, constant and collect all the terms corresponding to the different possible values of i_j. We then do the same for the other i_k's. After some sorting, we end up with

$$
\begin{aligned}
=&\tau\left[A^{(ij)}\right] + \sum_{s=1}^{\infty} k_s(\dot{V},\dots,V)\left(\tau\left[\frac{1}{z-H}\right]\right)^{s-1}\times\tau\left[A^{(ij)}\,\frac{1}{z-H}\right], \\
=&\tau\left[A^{(ij)}\right] + K_V\left(\tau\left[\frac{1}{z-H}\right]\right)\times\tau\left[A^{(ij)}\,\frac{1}{z-H}\right]. \qquad (4.8)
\end{aligned}
$$

It is is rather hard to justify this reordering a priori. However, starting from equation (4.8), we can retrace our steps and prove convergence that way.

The cumulant series K_V is a formal series, but in an appropriate neighborhood of 0 it converges absolutely to an holomorphic function. In [66], it was proven that the cumulants k_s of a bounded operator V do not grow faster than $(16\|V\|)^s$. The cumulant series thus converges in a neighborhood of 0 with a radius not less than $1/(16\|V\|)$.

The argument of K_V is the expectation value of the resolvent mapping $R(z)$. As $\tau[R(z)] \to 0$ when $|z| \to \infty$, we can be sure that an environment exists such that $|\tau[R(z)]| < 1/(16\|V\|)$. Likewise, in such an environment, the Neumann series of $\tau[R(z)]$ converges absolutely. Using Fubini's theorem we can now safely rearrange all terms in (4.8) to retrieve the earlier expression.

Iteration point We can reiterate the above calculation for the second term in (4.8) where the 'surplus' $A^{(ij)}$ is now replaced by $A^{(ij)}A$. Doing this once, gives us

$$\begin{aligned} n_{ij}(z) =& \tau\left[A^{(ij)}\right] + K_S\left(\tau\left[\frac{1}{z-H}\right]\right) \times \tau\left[A^{(ij)}A\right] + \\ &+ \left(K_S\left(\tau\left[\frac{1}{z-H}\right]\right)\right)^2 \times \tau\left[A^{(ij)}A\,\frac{1}{z-H}\right]. \end{aligned}$$

We can repeat this process an infinite amount of times, such that for sufficiently large $|z|$, it generates a convergent series and we obtain

$$n_{ij}(z) = \sum_{n=0}^{\infty} \tau\left[A^{(ij)}\left(K_V\left(\sum_k \mathbf{r}_{kk}(z)\right)A\right)^n\right], \tag{4.9}$$

where we also have used the identity,

$$\tau\left[\frac{1}{z-H}\right] = \sum_k \tau\left[(E_{kk}\otimes \mathbb{1}_{\mathcal{E}})\,\frac{1}{z-H}\right] = \sum_k \mathbf{r}_{kk}(z).$$

Expression (4.9) is tantamount to equating two Neumann series which again for large enough $|z|$ converge to

$$\mathbf{r}_{ij}(z) = \tau\left[(E_{ji}\otimes \mathbb{1}_{\mathcal{E}})\,\frac{1}{z\mathbb{1} - K_V(\sum_k \mathbf{r}_{kk}(z))\mathbb{1} - H_0}\right].$$

We can rewrite this equation into a more telling form by expanding out H_0 explicitly as the sum of $H_0^S \otimes \mathbb{1}_{\mathcal{E}}$ and $\mathbb{1}_{\mathcal{S}} \otimes H_0^E$,

$$\mathbf{r}_{ij}(z) = \tau\left[(E_{ji}\otimes \mathbb{1}_{\mathcal{E}})\,\frac{1}{z - K_V\left(\sum_k \mathbf{r}_{kk}(z)\right) - H_0^S\otimes\mathbb{1}_{\mathcal{E}} - \mathbb{1}_{\mathcal{S}}\otimes H_0^E}\right]. \tag{4.10}$$

Since by construction $H_0^S \otimes \mathbb{1}_{\mathcal{E}}$ and $\mathbb{1}_{\mathcal{S}} \otimes H_0^E$ are diagonal in the computational basis, the more complicated operator,

$$\frac{1}{z - K_V\left(\sum_k \mathbf{r}_{kk}(z)\right) - H_0^S\otimes\mathbb{1}_{\mathcal{E}} - \mathbb{1}_{\mathcal{S}}\otimes H_0^E},$$

is also diagonal in the computational basis. A first, direct consequence of this is that all off-diagonal matrix elements of $\mathbf{r}(z)$ are zero. Secondly, with obvious notational meaning, equation (4.10) can be rewritten as,

$$\mathbf{r}_{ij}(z) = \delta_{i,j}\,\frac{1}{d}\,\tau_{\mathcal{E}}\left[\frac{1}{z - K_V\left(\sum_k \mathbf{r}_{kk}(z)\right) - \epsilon_i - H_0^E}\right].$$

If we write the expectation under the functional $\tau_{\mathcal{E}}$ in terms of the probability measure of H_0^E, we can rework the previous equation as

$$\mathbf{r}_{ii}(z) = \frac{1}{d}\int d\mu_{H_0^E}(\lambda)\frac{1}{z - K_V\left(\sum_k \mathbf{r}_{kk}(z)\right) - \epsilon_i - \lambda}, \tag{4.11}$$

or

$$\mathbf{r}(z) = \frac{1}{d}\,\mathbb{E}\left[\frac{1}{z - K_V(\sum_k \mathbf{r}_{kk}(z)) - H_0}\right].$$

Uniqueness of solutions

To prove uniqueness of the solution of the above equations, it suffices to show that the trace of the solution, $r(z)$, is unique, since the $\mathbf{r}_{ii}(z)$ can all be calculated from this quantity $r(z) = \sum_k \mathbf{r}_{kk}(z)$ by formula (4.11). If we sum up all the $\mathbf{r}_{ii}(z)$ as in (4.10), we come up with an alternative form of the moment cumulant relation established in theorem 3.34,

$$r(z) = \tau\left[\frac{1}{z - K_V(r(z)) - H_0}\right].$$

The crucial point in arguing that this equation produces a unique solution, is the Earle-Hamilton theorem. As a reminder [67],

Theorem 4.3 (Earle-Hamilton)**.** *Let $\mathcal{D}$ be a nonempty domain in a complex Banach space X and let $h : \mathcal{D} \to \mathcal{D}$ be a bounded holomorphic function. If $h(\mathcal{D})$ lies strictly inside $\mathcal{D}$ (i.e., there is some $\epsilon > 0$ such that $B_\epsilon(h(x)) \subset \mathcal{D}$, whenever $x \in \mathcal{D}$, where $B_\epsilon(y)$ is the ball of radius ϵ about y), then h is a strict contraction in the Carathéodory-Riffen-Finsler metric ρ, and thus has a unique fixed point in $\mathcal{D}$. Furthermore, one has for all $x, y \in \mathcal{D}$ that $\rho(x, y) \geq m\|x - y\|$ for some constant $m > 0$, and thus $(h^n(x_0))_{n\in\mathbb{N}}$ converges in norm, for any $x_0 \in \mathcal{D}$, to this fixed point.*

-

At least on the domain $\mathcal{D} = \{w \,|\, |w| < 1/(16\|V\|)\}$, K_V is a bounded holomorphic function. If z is in an appropriate neighborhood of ∞, we can thus define a bounded, holomorphic map F_z on the domain $\mathcal{D}$ as

$$F_z(w) = \tau\left[\frac{1}{z - K_V(w) - H_0}\right], \quad \forall\, w \in \mathcal{D}.$$

The behavior of this map is dominated by the behavior of z; for large $|z|$, we can always find a constant c such that

$$|F_z(w)| \leq \frac{c}{|z|}, \quad \forall\, w \in \mathcal{D}.$$

For sufficiently large $|z|$, the map $K_V(w)$ thus maps the domain $\mathcal{D}$ strictly to its interior. According to the Earle-Hamilton theorem, F_z is then a strict contraction in the Carathéodory metric and we are guaranteed that on this domain our equations produce a unique solution. Moreover, this domain is compatible with the domain where the constructive part of our proof holds. So, the unique solution of the above fixed point equation is $r(z)$.

□

Remark 4.4. If we restrict the contents of theorem 4.2 to only the information it provides about the Neumann series $G_H(z)$ of $r(z)$, it becomes equivalent to the moment-cumulant relation established in theorem 3.34. On the probability space $(\mathcal{S} \otimes \mathcal{E}, \tau)$, this relation amounts to

$$z\, G_H(z) = 1 + K_H\left(G_H(z)\right).\, G_H(z), \tag{4.12}$$

where $G_H(1/z)$ is the moment series of the random variable H. Whereas theorem 4.2, restated in these quantities, provides the relation

$$G_H(z) = G_{H_0}\left(z - K_V(G_H(z))\right). \tag{4.13}$$

Suppose now that we can set $H_0 = 0$ for a moment. Then $G_{H_0}(z) = 1/z$ and $H = V$. Since $H_0 = 0$ is still free from V, the above relation carries through and we obtain

$$G_H = \frac{1}{z - K_H(G_H(z))},$$

which is equivalent to

$$z\, G_H(z) = 1 + K_H\left(G_H(z)\right).\, G_H(z),$$

the formulation of theorem 3.34.

Showing that (4.12) implies (4.13) is a simple application of the inverse function theorem on formal power series. As a formal power series $G_{H_0}(z)$ has an inverse $G_{H_0}^{\langle -1\rangle}$ under composition. If we now apply relation (3.17) for the random variable H_0 in $z = G_{H_0}^{\langle -1\rangle}(w)$, we get a relation between this inverse and K_{H_0},

$$K_{H_0}(w) = G_{H_0}^{\langle -1\rangle}(w) - \frac{1}{w}, \tag{4.14}$$

which holds on the level of formal power series. Using additivity of cumulant series for the sum $H = H_0 + V$, we can rewrite the relation (4.12) as

$$z\, G_H(z) = \left[G_{H_0}^{\langle -1\rangle}(G_H(z)) + K_V(G_H(z))\right] G_H(z), \tag{4.15}$$

which translates easily into the relation (4.13).

-

Resolving a solution

The proof of 4.2 suggests a rather convenient solution strategy for the set of equations (4.5). The map $F_z(w)$,

$$F_z(w) = \tau\left[\frac{1}{z - K_V(w) - H_0}\right], \quad |w| \leq \frac{1}{16\|V\|}$$

we used to prove uniqueness, can also be used to calculate the expected resolvents. By construction, this map is a contraction for suitably chosen z. By repeated application of this map to a w inside the domain $\mathcal{D}$ of this map, we get closer and closer to the fixed point of this map. This fixed point is for any suitable z equal to $r(z)$, which is the only ingredient we need to calculate the individual $\mathbf{r}_{kk}(z)$.

Most often, this convergence seems quite fast, even when started from rather silly values, far from the fixed point. Still, the fixed point procedure can be optimized by making use of the holomorphicity of the resulting resolvent functions. Suppose we would like to know the value of $r(z)$ along some Jordan curve Γ, parametrized by the variable t, running from $t = 0$ to $t = e$. It pays to spend rather a large amount of computational resources to find the fixed point starting in $z(t = 0)$. Since $r(z)$ is holomorphic along the curve Γ, $r(z(0))$ is rather close to $r(z(0 + dt))$ if dt is small. Hence, it makes a rather good starting point for the iteration procedure for $r(z(0 + dt))$ which will now converge very fast to the fixed point.

Holomorphic extensions

The equations in theorem 4.2 hold only in a neighborhood of ∞. Technically, this is sufficient to calculate any expectation of a holomorphic function of H. For any holomorphic function f, the expectation value of $f(H)$ can be calculated as

$$\mathbb{E}\left[f(H)\right]_{ij} = \frac{d}{2\pi i} \oint_{\Gamma} dz\, f(z)\, \mathbf{r}_{ij}(z), \tag{4.16}$$

where Γ is a Jordan curve encircling the spectrum of H. We can always choose this Jordan curve such that at any point on the curve we are in a neighborhood where the equations of theorem 4.2 hold. Still, since we can only calculate $r(z)$ numerically through the fixed point equation (4.16), the spatial extendedness of the curve Γ prevents a practical solution. If the function f behaves nicely around ∞, this can be mediated somewhat by using the conformal mapping $z \mapsto 1/z$,

$$\frac{d}{2\pi i} \oint_{\Gamma} dz\, f(z)\, \mathbf{r}_{ij}(z) = -\frac{d}{2\pi i} \oint_{\Gamma'} dz'\, z'^{-2} f\left(\frac{1}{z'}\right)\, \mathbf{r}_{ij}\left(\frac{1}{z'}\right),$$

where Γ' is now a Jordan curve around 0. For any point z' on the Jordan curve Γ' we can easily calculate $\mathbf{r}_{ij}(1/z')$ numerically through the fixed point equation, since $1/z'$ lies in an appropriate neighborhood of ∞.

It is, however, both possible and desirable to extend the validity of theorem 4.2 somewhat so that we can use more reasonable Jordan curves to calculate expectations without any conformal manipulations. We only argue the extension for the expected resolvent mapping $r(z)$. The extension for the conditionally expected resolvent mapping $\mathbf{r}(z)$ follows automatically.

Proof. The derivation leans heavily on various results in a paper by Maassen [68] and some general considerations for compactly supported measures. We can summarize[10] the necessary results by the following lemma,

Lemma 4.5. *Let V be a Hermitian operator in some C^*-algebra $\mathcal{A}$ and let τ be a state on this algebra such that $(\mathcal{A}, \tau)$ forms a probability space. On the open disc $\mathcal{D} \subset \mathbb{C}$, centered at 0, with radius $(6\|V\|)^{-1}$, the free cumulant series $K_V(w)$ converges to a bounded, holomorphic function. Moreover, K_V maps $\mathcal{D}^+ := \mathcal{D} \cap \mathbb{C}^+$ to $\mathcal{D}^+$ and $\mathcal{D}^- := \mathcal{D} \cap \mathbb{C}^-$ to $\mathcal{D}^-$.*

-

We can use the domains $\mathcal{D}^+$ and $\mathcal{D}^-$ to come up with an appropriate fixed point equation for $r(z)$ that holds whenever $|\operatorname{Im} z| > 6\|V\|$. As in the proof of theorem 4.2, we introduce a map $F_z(w)$ on the domain $\mathcal{D}^+ \cup \mathcal{D}^-$,

$$F_z(w) = \begin{cases} 0, & \text{if} \quad \dfrac{\operatorname{Im} z}{\operatorname{Im} w} \geq 0, \\ \tau\left[\dfrac{1}{z - K_V(w) - H_0}\right], & \text{if} \quad \dfrac{\operatorname{Im} z}{\operatorname{Im} w} < 0, \end{cases}$$

whenever $|\operatorname{Im} z| > 6\|V\|$. Since K_V maps $\mathcal{D}^\pm$ to $\mathcal{D}^\pm$, F_z likewise maps $\mathcal{D}^\pm$ to $\mathcal{D}^\pm$. Similar to a resolvent mapping, we have the very coarse estimates,

$$|F_z(w)| \leq \frac{1}{|\operatorname{Im} z|} < \frac{1}{6\|V\|}.$$

So, for every z for which we defined it, F_z is a bounded, holomorphic map on $\mathcal{D}^+ \cup \mathcal{D}^-$ which maps $\mathcal{D}^+$ and $\mathcal{D}^-$ to their respective interiors. According to the Earle-Hamilton theorem, F_z is thus a strict contraction and the fixed point equation $w = F_z(w)$ produces a unique solution.

Since $r(z)$ is a resolvent mapping, it must satisfy

$$|r(z)| \leq \frac{1}{|\operatorname{Im} z|},$$

which means that for $|\operatorname{Im} z| > 6\|V\|$, it lies within the domain $\mathcal{D}$ and in particular in one of the subsets $\mathcal{D}^+$ or $\mathcal{D}^-$. So $r(z)$ is a possible candidate for the fixed point of the map F_z on $\mathcal{D}^+ \cup \mathcal{D}^-$.

The condition $|\operatorname{Im} z| > 6\|V\|$ is not sufficient to argue that the Neumann series of $r(z)$ converges. As a consequence, the constructive part of the proof of theorem 4.2 fails and so the status of $r(z)$ as a solution of $w = F_z(w)$ on the domain $\mathcal{D}$ is tentative. Luckily, we can leverage the holomorphic nature of the fixed point equation to prove that any solution of $w = F_z(w)$ on $\mathcal{D}^+ \cup \mathcal{D}^-$ should be equal to $r(z)$.

[10] This is done in more detail in section B.1 of the appendix.

Suppose that for each z, we use as starting point for the fixed point iteration, a point $w^0(z) \in \mathcal{D}^{\pm}$ such that $w^0(z)$ is an holomorphic function of z and furthermore $\operatorname{Im} w^0(z) \,.\, \operatorname{Im} z < 0$. A canonical choice is the function $w^0(z) = 1/z$. From the explicit form of F_z,

$$w^1(z) := F_z(w^0(z)) = \tau \left[\frac{1}{z - K_V(w(z)) - H_0} \right],$$

it is evident that on the domain $\mathcal{D}^+ \cap \mathcal{D}^-$, the map $w^1 : z \mapsto F_z(w(z))$ is an holomorphic function of z and that the relation $\operatorname{Im} w^0(z) \,.\, \operatorname{Im} z < 0$ propagates to $\operatorname{Im} w^1(z) \,.\, \operatorname{Im} z < 0$. By induction, any w^n,

$$w^n(z) := F_z((w^{n-1}(z)),$$

is then a holomorphic function of z and the relation $\operatorname{Im} w^n(z) \,.\, \operatorname{Im} z < 0$ holds. For any z, $w^n(z)$ tends to the unique solution of the fixed point equation $w = F_z(w)$, so with obvious notational implications, we can denote this solution as $w^\infty(z)$. As a function of z, w^∞ has the same properties as its older brothers and sisters, namely $w^\infty(z)$ is a holomorphic function of z and $\operatorname{Im} w^\infty(z) \,.\, \operatorname{Im} z < 0$

For large $|z|$, the constructive part of our proof still holds and there $w^\infty(z)$ is constructed as a convergent series in z, equal to the Neumann series of the expected resolvent mapping $r(z)$. Since the Neumann series of $r(z)$ and thus also $w^\infty(z)$ extends uniquely to an holomorphic function on $\mathbb{C}\backslash\mathbb{R}$, the solution to the fixed point equation $w = F_z(w)$ is everywhere on $\mathcal{D}^+ \cup \mathcal{D}^-$ equal to $r(z)$. So, not only is the equation,

$$r(z) = \tau \left[\frac{1}{z - K_V(r(z)) - H_0} \right],$$

valid whenever $|\operatorname{Im} z| > 6\|V\|$, but $r(z)$ is the unique solution of the equation $w = F_z(w)$. This solution can be found through iterating the associated map F_z.

By itself, this extension of theorem 4.2 is seemingly not enough to throw a Jordan curve around the spectrum of H. To do that, we need more information on how the fixed point equation behaves close to the real axis, or at least closer than $6\|V\|$. Since K_V is bounded by some number $c > 0$, we could repeat the above argument, but replace any requirement $x > 6\|V\|$ by $x > \|H_0\| + 6\|V\| + c$. Unfortunately, good bounds on K_V, so small values of c, are hard to find, at least in general. In specific situations, finding the correct bound is usually rather trivial. Furthermore, on general grounds, we can always find $r(z)$ for z on the lines $[\pm\|H\| + 6I\|V\|, \pm\|H\| - 6I\|V\|]$ by analytically continuing the solutions for $|\operatorname{Im} z| > 6\|V\|$. So, in effect, this extension reduces the needed contour for calculating expectations to a rather tight rectangle enclosing the spectrum of H.

□

It is this side effect of the map F_z which makes theorem 4.2 a valid and convenient tool for calculations. Without this, and also in the case that K_V does not extend to a Herglotz function on a sizeable domain, we would be left to calculate

integrals over some very extended Jordan curves in a neighborhood of ∞ when executing expectations. In the absence of such terminal cases, theorem 4.2 can be read as:

Theorem 4.6. *(Alternative form) Let H be the Hamiltonian of a dynamical model as proposed in section 4.1.2, so that H can be written as $H_0 + V$, where V is free from H_0 in the probability space $(\mathcal{S} \otimes \mathcal{E}, \tau)$. ~~In a neighborhood of ∞~~ The matrix elements of the renormalized expected resolvent $\mathbf{r}(z)$ can be calculated as,*

$$\mathbf{r}_{ij}(z) = \delta_{i,j} \frac{1}{d} \int d\mu_{H_0^E}(\lambda) \frac{1}{z - \epsilon_i - \lambda - K_V\left(r(z)\right)}, \quad \forall\, z \; s.t. \; |Im\ z| > 6\|V\|,$$

where K_V is the cumulant series of V and $\mu_{H_0^E}$ the spectral measure associated to the environmental part of the non-interacting hamiltonian H_0 and $r(z)$ is the unique solution of the self-consistent equation*,*

$$r(z) = \tau \left[\frac{1}{z - K_V(r(z)) - H_0} \right], \quad \forall\, z \; s.t. \; |Im\ z| > 6\|V\|.$$

Alternatively, these equations can be written as,

$$\mathbf{r}_{ij}(z) = \frac{1}{d} \left(\mathbb{E} \left[\frac{1}{z - H_0 - K_V(\sum_k \mathbf{r}_{kk}(z))} \right] \right)_{ij}.$$

-

Infinitely divisible distributions

In some cases, the cumulant series extends to an holomorphic function on $\mathbb{C}\backslash\mathbb{R}$. When this happens, the requirement on z in theorem 4.6 reduces to Im $z \neq 0$, which is almost nice enough to open a bottle of champagne.

The operators for which the cumulant series extends to a Herglotz function on $\mathbb{C}\backslash\mathbb{R}$ can be characterized in full. They correspond to the so-called $\boxplus$-infinitely divisible distributions.

Definition 4.7 (Infinitely divisible distributions)**.** A compactly supported measure μ on the real line is said to be $\boxplus$-*infinitely divisible* if for each $n \in \mathbb{N}$, there exists a compactly supported μ_n on the real line such that,

$$\mu = \underbrace{\mu_n \boxplus \cdots \boxplus \mu_n}_{n \text{ times}}.$$

-

The infinitely divisible distributions are a common sight in free probability because they provide an alternative to the classical semigroup structure of regular convolution. Any $\boxplus$-infinitely divisible distribution has a corresponding $\boxplus$-semigroup structure;

Definition 4.8. A one-parameter family $(\mu_t)_{t\geq 0}$ of compactly supported measures on the real line is called a $\boxplus$-semigroup if $\mu_s \boxplus \mu_t = \mu_{s+t}$ for all $t, s \geq 0$.

-

The following theorem not only cements this correspondence, but also identifies the cumulant series associated to such $\boxplus$-infinitely divisible distributions,

Theorem 4.9. *For a compactly supported measure μ on the real line, the following properties are equivalent,*

1. *μ is $\boxplus$-infinitely divisible.*
2. *There exists a w^*-continuous $\boxplus$-semigroup $(\mu_t)_{t\geq 0}$ such that $\mu_1 = \mu$.*
3. *The cumulant series K_μ extends to a Herglotz function on $(\mathbb{C}\backslash\mathbb{R}) \cup [-a, a]$, for some $a > 0$.*

If the above conditions hold, then,

$$K_{\mu_t}(z) = tK_\mu(z), \quad t \geq 0. \tag{4.17}$$

-

Proof. A proof of this theorem can be found in [39].

□

The above theorem clearly identifies the $\boxplus$-infinitely divisible distributions as the prime beneficiaries of theorem 4.6. In truth, theorem 4.6 has been somewhat tailored to suit exactly these types of distributions. There are quite a number of conjectures lying in between theorem 4.2 and theorem 4.6 that would be suitable to more general classes of distributions.

Infinitely divisible distributions are more than a mathematical convenience. They are stable attractors for the free convolution and the subject of various central limit theorems. In particular, the ever present semicircle laws are infinitely divisible distributions which is the reason for their appearance in theorem 4.1.

Remark 4.10. Above, we have indicated the similarities between theorem 4.2 (4.6) and theorem 3.34. Since we have put a great deal of effort in proving this newly minted theorem 4.2, it is perhaps a good idea to point out also the dissimilarities between the two moment-cumulant relations.

- The relations in theorem 4.2 are strictly speaking not moment-cumulant relations. Instead, they formulate a calculation strategy for the expected resolvent mapping of the operator H, provided we know the holomorphic function K_V. The object $\mathbf{r}(z)$ is not at all a moment series. It carries a lot more structure than the simple formal series $G_H(z)$ of theorem 3.34, it is a holomorphic function on $\mathbb{C}\backslash\Sigma(H)$ and a twisted Herglotz function (it maps $\mathbb{C}^+$ onto $\mathbb{C}^-$ and vice-versa). Correspondingly, theorem 4.2 relates more than just the coefficients of two power series; it provides connections between two holomorphic functions.

- It is possible to equip theorem 3.34 with a similar holomorphic component as our theorem 4.2. Per remark 4.4, this can be easily achieved by going through the proof of theorem 4.2 for $r(z)$ with H_0 set to zero.

  Even then, the two theorems are not equal in content. The main reason we developed theorem 4.2 is that it does not use up all information about our free random variables in one shot. For any holomorphic function f, both theorem 4.2 and a modified version of theorem 3.34 allow us to calculate the expectation value $\tau\left[f(H)\right]$. Only theorem 4.2 provides the necessary information to calculate something like $\tau\left[H_0\, f(H)\right]$.

-

4.3.2 Spectral properties of free convolution

The main universal physical features of free interactions that we have identified, or rather will identify in sections 4.4 and 4.6, follow from the spectral properties of free convolution. As was touched upon in example 3.37, free convolution tends to smear out atomic measures, much more so than its classical cousin. We will see in sections 4.4 and 4.6 why this smearing is so important. For now we content ourselves with establishing that such smearing occurs almost surely.

The most general result on this, that we are aware of, is by Belinschi [69],

Theorem 4.11 (Spectral features)**.** *Let μ, ν be two Borel probability measures on $\mathbb{R}$, neither of them a point mass. Then*

(1) *The point $a \in \mathbb{R}$ is an atom of the measure $\mu \boxplus \nu$ if and only if there exist $b, c \in \mathbb{R}$ such that $a = b + c$ and $\mu(\{b\}) + \nu(\{c\}) > 1$. Moreover, $(\mu \boxplus \nu)(\{a\}) = \mu(\{b\}) + \nu(\{c\}) - 1$.*

(2) *The absolutely continuous part of $\mu \boxplus \nu$ is always nonzero, and its density is holomorphic wherever positive and finite. More precisely, there exists an open set $U \subseteq \mathbb{R}$ so that the density function $f(x) = \frac{d(\mu \boxplus \nu)^{ac}(x)}{dx}$ with respect to the Lebesgue measure in the real line is holomorphic on U and $(\mu \boxplus \nu)^{ac}(\mathbb{R}) = \int_U f(x)dx$.*

(3) *The singular continuous part of $\mu \boxplus \nu$ is zero.*

-

4.3.3 A free toy model specter

As promised, we illustrate the general results in this chapter by applying them to the toy model introduced in section 4.2. Recall that in our free toy model, the interaction V is assumed to be a semicircular element with zero mean and a set

variance v. For such semicircular elements, the cumulant series is the very simple function

$$k_V(z) = v^2\, z.$$

Although we have already argued extensively why we use semicircular variables for the interaction in our toy model, a more practical reason should now be apparent. The cumulant series of semicircular elements extend very trivially to Herglotz functions on $\mathbb{C}$ and so theorem 4.6 can be used instead of theorem 4.2 to analyze this model. For our toy model, the equations in theorem 4.6 reduce to

$$\mathbf{r}_{ij}(z) = \delta_{i,j} \frac{1}{2} \int d\mu_{H_0^E}(\lambda)\, \frac{1}{z - \epsilon_i - v^2\, r(z) - \lambda},$$

and

$$r(z) = \int d\mu_{H_0}(\lambda)\, \frac{1}{z - v^2\, r(z) - \lambda}.$$

The solutions of these equations also depend on our choice of H_0, which sets the energy levels in the unperturbed system and environment. For the uniform environmental spectrum in our toy model, this results in

$$\mathbf{r}_{ij}(z) = \delta_{i,j}\, \frac{1}{4h} \int_{-h}^{h} d\lambda\, \frac{1}{z + (-1)^i\, \epsilon - v^2\, r(z) - \lambda},$$

and

$$r(z) = \frac{1}{4h} \int_{-h}^{h} d\lambda \left(\frac{1}{z + \epsilon - v^2\, r(z) - \lambda} + \frac{1}{z - \epsilon - v^2\, r(z) - \lambda} \right).$$

The integrals in these expressions can be explicitly carried out, which yields,

$$\mathbf{r}_{ij}(z) = \delta_{i,j}\, \frac{1}{2h}\ \operatorname{arccoth}\left(\frac{z + (-1)^i \epsilon - v^2\, r(z)}{h} \right),$$

and

$$r(z) = \frac{1}{2h}\ \left(\operatorname{arccoth}\left(\frac{z + \epsilon - v^2\, r(z)}{h} \right) + \operatorname{arccoth}\left(\frac{z - \epsilon - v^2\, r(z)}{h} \right) \right). \quad (4.18)$$

Although the non-algebraic nature of the self-consistent equation (4.18) prevents a description of $r(z)$ in terms of elementary functions, the full form of $r(z)$ on $\mathbb{C}\backslash\Sigma(H)$ can be recovered numerically by the iteration procedure proposed in section 4.3.1. By using Stone's formula (theorem 3.50) we can then explicitly compute the probability density function of the operator H both under the state τ and the conditional expectation $\mathbb{E}$.

Remark 4.12. Equivalently, for $r(z)$ we could have started our analysis of this model from the original moment-cumulant relation (3.17) in theorem 3.34 directly to reduce the problem to a self-consistent equation of the form

$$z\, r(z) = 1 + r(z) K_H\left(r(z)\right),$$

or

$$r(z) = \frac{1}{z - K_H\left(r(z)\right)} = \frac{1}{z - v^2\, r(z) - K_{H_0}\left(r(z)\right)}.$$

This last equation looks deceivingly simple. The difficulty lies in calculating the cumulant function of H_0. Although we know the spectrum of H_0 explicitly, $K_{H_0}(w)$ cannot be calculated algebraically, only numerically. The moment series $G_{H_0}(z)$ on the other hand can be computed algebraically rather straightforwardly and so (4.5) more easily reduces to an explicit fixed point equation than the original moment-cumulant relation of theorem 3.34.

-

Below, figures 4.1 and 4.2 detail a few numerical examples of these probability density functions. Figure 4.1 shows the spectral distribution of the global Hamiltonian H under the state τ. Figure 4.2 shows the imaginary part of $\mathbf{r}_{11}(z)$ on the real axis. Because of the rescaling of $\mathbf{r}$, the graphs in figure 4.2 do not correspond to probability distributions. The integral over the real axis of these functions is not 1, but 1/2.

The parameters in the examples are specifically chosen to showcase how the pdf's change with increasing parameter strength, though the general features of these examples are mimicked for other parameter ranges as well.

Notice especially how all shown probability density functions are absolutely continuous in line with theorem 4.11. The only realistic cases where the pdf's fail to be absolutely continuous are the terminal cases where either $V = 0$ or the spectrum of H_0^E contains isolated eigenvalues.

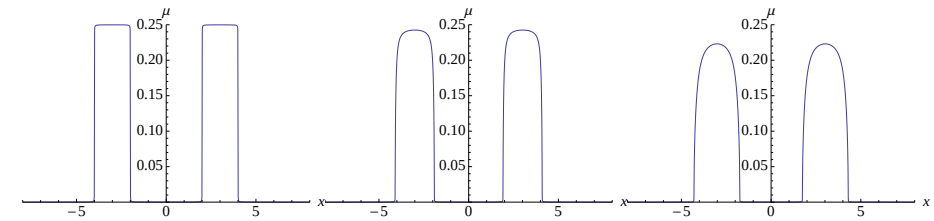
4.3.4 Local equilibrium states

In general, the construction of equilibrium states for infinite systems is a rather complicated problem. Even the definition of what an equilibrium state entails is slightly arbitrary in such systems. For finite systems, the situation is much better. Although a myriad of characterizations exist, they are all equivalent and point out that the equilibrium states of a finite system are exactly those with a density matrix ρ_β of Gibbs form,

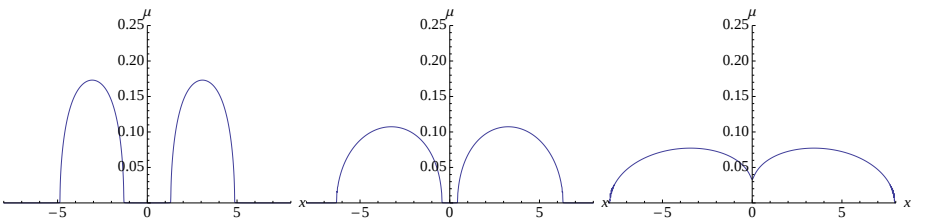
$$\rho_\beta = \frac{e^{-\beta H}}{\operatorname{Tr} e^{-\beta H}},$$

where β is an inverse temperature and H is the Hamiltonian governing the system.

Loosely stated, the problem with characterizing equilibrium states for infinite systems stems from the fact that the above expression is often not well defined for

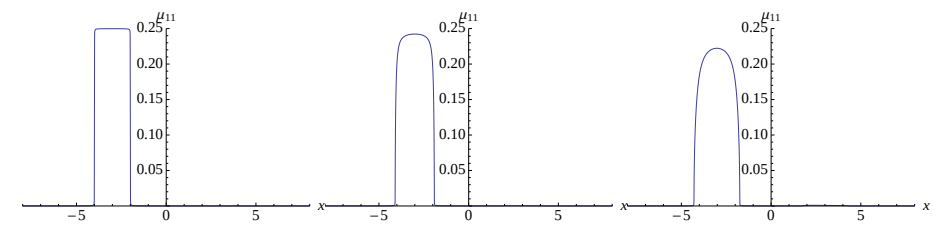


(a) $v = 0$ (b) $v = 1/4$ (c) $v = 1/2$

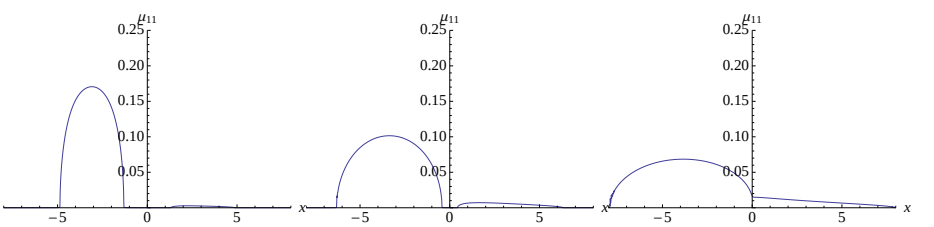


(d) $v = 1$ (e) $v = 2$ (f) $v = 3$

Figure 4.1: The figure shows the probability density measure of the Hamiltonian H under the state τ for successively larger values of the coupling parameter v. The parameter ϵ is set to 3 and $h = 1$.



(a) $v = 0$ (b) $v = 1/4$ (c) $v = 1/2$



(d) $v = 1$ (e) $v = 2$ (f) $v = 3$

Figure 4.2: The figure shows the imaginary part of $\mathbf{r}_{11}(z)$ on the real axis for successively larger values of the coupling parameter v. The parameter ϵ is set to 3 and $h = 1$. $\mathbf{r}_{22}(x)$ is the mirror image of $\mathbf{r}_{11}(x)$ under reflection over the vertical axis.

such systems. A partial solution to this problem is to start with a small, finite subsystem and then take a limit in ever expanding system sizes, i.e. we consider

$$\lim_{|\Lambda|\to\infty} \frac{e^{-\beta H_\Lambda}}{\operatorname{Tr} e^{-\beta H_\Lambda}},$$

where Λ denotes some local restriction of the infinite algebra and H_Λ the restriction of the global Hamiltonian H to the subsystem Λ. Even in this approach, the existence and uniqueness of such an object is debatable. Rather than repeat all the results obtained on this subject, we simply assume that, for the systems we are studying, the limit

$$\lim_{|\Lambda|\to\infty} \frac{e^{-\beta H_{0,\Lambda}}}{\operatorname{Tr} e^{-\beta H_{0,\Lambda}}},$$

is well-defined for the non-interacting system governed by the Hamiltonian H_0, and provides a unique notion of equilibrium states. We further assume that the nature of the limit is compatible with taking the limit for a converging series of interaction terms V_n which leads to our free interaction term V. Let us state this somewhat more precisely. Suppose that $(V_n)_{n\in\mathbb{N}}$ is a series of bounded operators which converges to the free random variable V,

$$\lim_{n\to\infty} V_n = V,$$

and that a compatible division of the global system $S + E$ exists, such that for any n, there exists a finite global system $S + E_n$ such that $\mathcal{E}_n \subset \mathcal{E}$ and

$$\lim_{n\to\infty} \mathcal{S} \otimes \mathcal{E}_n = \mathcal{S} \otimes \mathcal{E}.$$

Suppose furthermore that for every finite system we can define a restriction $H_{0,n}$ of the Hamiltonian H_0 such that in the limit the resulting series converges to H_0 and

$$\lim_{n\to\infty} \frac{e^{-\beta H_{0,n}}}{\operatorname{Tr}_n e^{-\beta H_{0,n}}} \tag{4.19}$$

is well-defined and results in a unique notion of equilibrium states.

Since the series $(V_n)_n$ is composed of bounded operators and converges to a bounded operator, the limit

$$\lim_{n\to\infty} \frac{e^{-\beta(H_{0,n}+V)}}{\operatorname{Tr}_n e^{-\beta(H_{0,n}+V)}}$$

will also converge and thus defines a unique set of equilibrium states for the interacting system.

Although theorem 4.2 can be extended to calculate the global equilibrium states of the combined system $S + E$ under these conditions, doing so would be rather futile since we have defanged the problem to such an extend that no meaningful

information about the global system would be gained. Furthermore, in order to do so, we would have to explicitly define the operator form of H_0^E which in many cases will lead to a conflict with the assumptions made in this section or to situations which are already known.

The local restrictions of the proposed equilibrium states (4.19) on the other hand, still carry sufficient meaning. Loosely stated, we will fill in the dots in: "*If the global algebra $\mathcal{S} \otimes \mathcal{E}$ admits a unique notion of equilibrium states in the sense of* (4.19)*, then the local restrictions look like ...*".

Of course, we still have to calculate these local restrictions. For any restriction $S + E_n$, we can define a local state on the system S by the density matrix

$$\mathrm{Tr}_{\mathcal{E}_n}\left[\frac{e^{-\beta(H_{0,n}+V)}}{\mathrm{Tr}_n\, e^{-\beta(H_{0,n}+V)}}\right],$$

where $\mathrm{Tr}_{\mathcal{E}_n}$ is the partial trace over the environment E_n. The trace operation on these finite restrictions also naturally give rise to the tracial states $\tau_{\mathcal{E}_n} := \frac{1}{n}\,\mathrm{Tr}_{\mathcal{E}_n}$ and $\tau_n := \frac{1}{d\times n}\,\mathrm{Tr}_n$. The local restrictions can thus be restated as

$$\frac{1}{d}(\mathrm{id}\otimes\tau_{\mathcal{E}_n})\left[\frac{e^{-\beta(H_{0,n}+V)}}{\tau_n\left[e^{-\beta(H_{0,n}+V)}\right]}\right],$$

where d is the dimension of the system S. In the limit of $n \to \infty$, these density matrices converge to our desired equilibrium density matrices,

$$\rho_\beta = \lim_{n\to\infty} \frac{1}{d}(\mathrm{id}\otimes\tau_{\mathcal{E}_n})\left[\frac{e^{-\beta(H_{0,n}+V)}}{\tau_n\left[e^{-\beta(H_{0,n}+V)}\right]}\right]. \tag{4.20}$$

The further analysis of such equilibrium states will obviously depend very much on the specific nature of the interaction and the probability measure of H_0. Because of our earlier assumptions, this limit is no longer very problematic. The choice of a free interaction terms means that the only information we need about the Hamiltonian H_0 is the limiting probability measure associated to it. No matter the form of this measure, we can always approximate it by a convergent series of compactly supported measures. So, in practice, taking this limit is somewhat pedantic. For any given, non-compact probability measure, we can approximate the solution arbitrarily well by cutting off the measure at some very distant point and calculate the Gibbs state for that, now compactly supported, measure.

Universal properties of the equilibrium states

Preferred basis The local restrictions of the Gibbs density matrices are all diagonal in the computational, or energy, basis of the system S. This is a direct consequence of theorem 4.2. To see how exactly, we restrict ourselves for a moment to the case where H_0 is a bounded operator. In such a case, we can forget about

taking the limit and simply state that

$$\rho_\beta = \frac{1}{d}\,\frac{1}{\tau\left[e^{-\beta H}\right]}\,\mathbb{E}\left[e^{-\beta H}\right].$$

Such quantities can easily be calculated using theorem 4.2. Recall that according to the holomorphic functional calculus in section 3.6, both the denominator and the numerator can be rewritten in terms of the (conditionally) expected resolvent mapping as,

$$\mathbb{E}\left[e^{-\beta H}\right] = \frac{1}{2\pi i}\int_\Gamma dz\, e^{-\beta z}\,\mathbb{E}\left[\frac{1}{z-H}\right] = \frac{d}{2\pi i}\int_\Gamma dz\, e^{-\beta z}\,\mathbf{r}(z),$$
$$\tau\left[e^{-\beta H}\right] = \frac{1}{2\pi i}\int_\Gamma dz\, e^{-\beta z}\,\tau\left[\frac{1}{z-H}\right] = \frac{1}{2\pi i}\int_\Gamma dz\, e^{-\beta z}\,r(z),$$

where Γ is some suitable chosen set of Jordan curves which encloses the spectrum of H. Combined, this gives us an expression for ρ_β of

$$\rho_\beta = \frac{\int_\Gamma dz\, e^{-\beta z}\,\mathbf{r}(z)}{\int_{\Gamma'} dz'\, e^{-\beta z'}\,r(z'),} \tag{4.21}$$

As $\mathbf{r}_{ij}(z) = 0$ if $i \neq j$, we immediately obtain that $(\rho_\beta)_{ij} = 0$ if $i \neq j$. Since this result holds for all possible Hamiltonians considered, this holds true in any limiting situation as well.

Diagonal entries The diagonal matrix elements of the equilibrium density matrices depend on the specific properties of the interaction, the type of environment and the Bohr spectrum of the system itself. Somewhat unremarkable, the infinite temperature Gibbs states are not affected. Only the total expected energy in these states is affected. The expected energy is shifted by the mean of the interaction V.

The remaining equilibrium states can only be described quantitatively in more detail than (4.21) by considering specific models. The qualitative behavior on the other hand seems to be somewhat universal. In particular, an interaction of semicircle type provides a first-order approximation to the equilibrium states of more general interaction types, in line with the comments made in section 4.3.3. The figure below shows the behavior of the diagonal matrix elements of the equilibrium states for the example in section 4.3.3.

4.4 Dynamics of freely interacting systems

Perhaps the most physically thrilling part of this chapter is the prospect of describing the dynamical properties of the reduced density matrix $\sigma(t)$ in terms of simple physical quantities. Macroscopic bounds on the interaction lead in a very natural

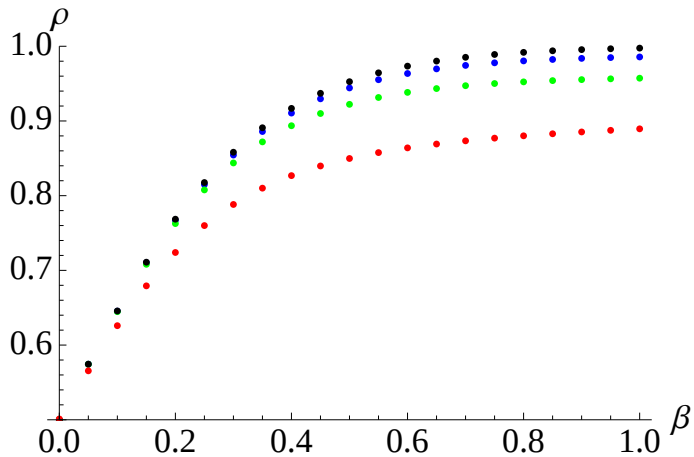


Figure 4.3: Any reduced equilibrium state is a convex combination of the two eigenstates of H_0^S. This figure shows the presence of the ground state in such a convex combination in terms of the rescaled inverse temperature $\beta/2\epsilon$. From top to bottom, the curves are plotted for $v = 0$, $v = 1$, $v = 2$, $v = 4$.

way to a restriction of the possible interactions to those which are free from the uncoupled Hamiltonian H_0 in the probability space $(\mathcal{S} \otimes \mathcal{E}, \tau)$.

The introduction of free interactions allows us to 'trace out' the interaction term V for this problem. This results in an integral equation which describes the time evolution of the reduced density matrix for the system S.

The initial state and the unperturbed Hamiltonian H_0 enter this equation as operators. In contrast, the equation only depend on the interaction term V in terms of its cumulant series, which is a scalar function. The macroscopic contraints on the interaction are all encoded in this function.

The resulting integral equation is still a very complex object. For many cases, the problem remains intractable. This is not a deficit of the model, but rather represent our refusal to neglect the influence of the system on the environment. In addition, in its most general form, the integral equation also allows for environments which are initially not in equilibrium. Since the environment is assumed to be an infinite system, the resulting dynamics of the environment remains intractable even if no coupling were to be present.

Only if we assume that the initial state of the environment is invariant under the uncoupled dynamics, does the problem reduce to a tractable integral equation. The coupling between the system and environment can still influence the state of the environment, but violent corrections because of the infinite Hamiltonian H_0 are eliminated. Only perturbations resulting from the interplay of the interaction V and H_0 are then important.

The resulting integral equation in such a situation is still sensitive to memory effects. This makes solving the equation a tractable, but still complicated problem.

4.4.1 Resolving the reduced dynamics

The modified moment-cumulant relations obtained in section 4.3 can be used to calculate the reduced density matrix,

$$\sigma(t) = \mathbb{E}\left[e^{itH}(\sigma(0)\otimes \mathsf{E})e^{-itH}\right],$$

if we impose the additional restriction that the interaction V is also taken to be free from the initial state of the environment. This condition is in particular fulfilled by the equilibrium states of the environment, as well as by the eigenstates of the Hamiltonian H_0^E.

Using holomorphic functional calculus, we can rewrite $\sigma(t)$ in terms of the resolvent of the Hamiltonian as

$$\sigma(t) = -\frac{1}{4\pi^2}\oint_{\Gamma} dz_1 dz_2\, e^{it(z_1-z_2)}\,\mathbb{E}\left[\frac{1}{z_1-H}\,(\sigma(0)\otimes\mathsf{E})\,\frac{1}{z_2-H}\right], \tag{4.22}$$

where Γ is some suitably[11] chosen set of Jordan curves encircling the spectrum of H.

A similar technique as was used in section 4.3 to calculate the reduced resolvent mapping of H can then be used to calculate explicitly the two-point function $\mathbf{r}(z_1, z_2)$,

$$\mathbf{r}(z_1,z_2) := \mathbb{E}\left[\frac{1}{z_1-H}\,(\sigma(0)\otimes\mathsf{E})\,\frac{1}{z_2-H}\right].$$

As in the case of the Hamiltonian specter, it is convenient to introduce a specific notation for the trace of $\mathbf{r}(z_1, z_2)$,

$$r(z_1,z_2) := \mathrm{Tr}\;\mathbb{E}\left[\frac{1}{z_1-H}\,(\sigma(0)\otimes\mathsf{E})\,\frac{1}{z_2-H}\right].$$

To make the two-point function more amenable to our probabilistic framework, we need to translate it to the probability space $(\mathcal{S}\otimes\mathcal{E},\tau)$,

$$\mathbf{r}_{ij}(z_1,z_2) = \tau\left[(E_{ji}\otimes\mathbb{1}_{\mathcal{E}})\frac{1}{z_1-H}\,(\mathsf{S}\otimes\mathsf{E})\,\frac{1}{z_2-H}\right].$$

As was indicated in section 4.3, the rescaled expectation $r(z)$ is an essential ingredient in this reduced description. The following lemma describes how the two-point function $\mathbf{r}(z_1, z_2)$ can be written as a function of the (one-point) function $r(z)$.

[11] In light of the calculations below, care should be taken that the contour used for the integral over z_1 is completely enclosed by the contour used for the integral over z_2.

Lemma 4.13. *Let H be the Hamiltonian of a dynamical model as proposed in section 4.1.2, so that H can be written as $H_0 + V$, where V is free from H_0 in the probability space $(\mathcal{S} \otimes \mathcal{E}, \tau)$. If $|Im\ z_1| > 6\|V\|$ and $|Im\ z_2| > 6\|V\|$, the two point function $\mathbf{r}(z_1, z_2)$,*

$$\mathbf{r}(z_1, z_2) = \mathbb{E}\left[\frac{1}{z_1 - H}\,(\sigma(0) \otimes \mathsf{E})\,\frac{1}{z_2 - H}\right],$$

is amenable to a description in terms of the rescaled conditionally expected resolvent mapping of H,

$$\begin{aligned}\mathbf{r}(z_1, z_2) &= \frac{\mathbf{r}(z_1) - \mathbf{r}(z_2)}{z_2 - z_1} \times \frac{K_V\left(r(z_1)\right) - K_V\left(r(z_2)\right)}{r(z_1) - r(z_2)} \\ &\times \mathrm{Tr}\,\mathbb{E}\left[\frac{1}{z_1 - K_V(r(z_1)) - H_0}(\sigma(0) \otimes \mathsf{E})\frac{1}{z_2 - K_V(r(z_2)) - H_0}\right] \\ &+ \mathbb{E}\left[\frac{1}{z_1 - K_V(r(z_1)) - H_0}(\sigma(0) \otimes \mathsf{E})\frac{1}{z_2 - K_V(r(z_2)) - H_0}\right].\end{aligned} \tag{4.23}$$

Proof. The proof of this lemma can be found in section B.2 of the appendix. The techniques used are similar to those used in the proof of theorem 4.2, but with some additional technical complexities. The interested reader is certainly invited to read through the proof, since calculations of this nature are usually not considered in free probability theory.

□

Lemma 4.13 allows us to write down a set of explicit dynamical equations for the reduced density matrx $\sigma(t)$. Although technically a corollary to lemma 4.13, we state the following as a theorem,

Theorem 4.14. *Let H be the Hamiltonian of a dynamical system as proposed in section 4.1.2, so that H can be written as $H_0 + V$, where V is free from H_0 in the probability space $(\mathcal{S} \otimes \mathcal{E}, \tau)$. At any time t, the reduced state on the system S is described by the density matrix $\sigma(t)$, which can be calculated as*

$$\begin{aligned}\sigma(t) = \oint_\Gamma dz_1\, dz_2\, e^{it(z_1 - z_2)}\ &\frac{\mathbf{r}(z_1) - \mathbf{r}(z_2)}{z_2 - z_1} \times \frac{K_V\left(r(z_1)\right) - K_V\left(r(z_2)\right)}{r(z_1) - r(z_2)} \\ &\times \mathrm{Tr}\,\mathbb{E}\left[\frac{1}{z_1 - K_V(r(z_1)) - H_0}(\sigma(0) \otimes \mathsf{E})\frac{1}{z_2 - K_V(r(z_2)) - H_0}\right] \\ + \oint_\Gamma dz_1\, dz_2\, e^{it(z_1 - z_2)}&\mathbb{E}\left[\frac{1}{z_1 - K_V(r(z_1)) - H_0}(\sigma(0) \otimes \mathsf{E})\frac{1}{z_2 - K_V(r(z_2)) - H_0}\right].\end{aligned}$$

Since we can only calculate $r(z)$ numerically, the solutions to the equations in theorem 4.14 can likewise be calculated only numerically. This limitation is inherent to the free model. The dynamical behavior of our model systems simply cannot be described in algebraic terms.

As a consequence, it is rather difficult to prove any type of general results about the dynamics of this model. At first, this struck us as a rather disappointing finish, especially considering the mathematical effort needed to derive theorem 4.14.

After the initial numerical analysis of the dynamical equations, this disappointment dissipated somewhat. As we will illustrate in the analysis of the free toy model, the dynamical behavior of our free models has a very rich structure which cannot be summarized in any succinct way. Simply because there is no universal behavior to be summarized. A model system can be driven to an equilibrium state by the interaction or not. If it is drive to equilibrium, this convergence can be exponential, follow a power law, or the system can undergo both exponential and power law decay at various time intervals.

In hindsight, one could say that this result was to be expected considering the different scales which we hope to describe with our models. Weak or strong interactions, big or small systems, cold or hot environments; at least on a mathematical level, all of these situations are described by the same set of equations.

It is however possible that these different situations can be somewhat grouped together in terms of their dynamical behavior. Unfortunately, our analysis of these models has not progressed far enough to attempt such a feat. For the moment, we can only illustrate theorem 4.14 by looking at some specific examples and analyzing the behavior of those models.

Remark 4.15. At the end of section 4.1.1, we listed some desirable qualities for a description of the reduced dynamics of a system. Theorem 4.14 allows us to now check of the four points we suggested there.

- The use of free random variables cements many of the otherwise unknowable parameters in a model interaction. We only need to specify certain macroscopic observables to fully determine the necessary information in our model. Hence, our model is indeed easy to construct.

- Since we are dealing with infinite environments, any microscopic change in the interaction or environment is drowned out by the predominant spectral features of the model and do not change the dynamical behavior of the system.

- Macroscopic perturbations can influence the behavior of a system. To deal with those types of perturbations, it is sufficient to simply change the parameters in the original model slightly. These perturbations can thus be handled with the same ease as the original model.

- Although the equations in theorem 4.6 and theorem 4.14 scale only with

the size of the system, we cannot claim that the resulting dynamics is easy to calculate, at least, not algebraically. Numerically, the computation of the reduced dynamics can be calculated quite fast and the procedure scales especially well to large system sizes.

4.4.2 Dynamical behavior of a two-level system

As for the Hamiltonian specter, we illustrate the general formula for the reduced dynamics by some numerical results on the free toy model. The cumulant series K_V has the exceptionally simple form

$$K_V(z) = v^2 z.$$

The general form of the reduced dynamics thus reduced to,

$$\begin{aligned}\sigma(t) = &-\frac{1}{4\pi^2}\oint_\Gamma dz_1\, dz_2 e^{it(z_1-z_2)} \\ &v^2\frac{\mathbf{r}(z_1)-\mathbf{r}(z_2)}{z_2-z_1}\times \operatorname{Tr}\mathbb{E}\left[\frac{1}{z_1-v^2r(z_1)-H_0}(\sigma(0)\otimes \mathsf{E})\frac{1}{z_2-v^2r(z_2)-H_0}\right] \\ &+\mathbb{E}\left[\frac{1}{z_1-v^2r(z_1)-H_0}(\sigma(0)\otimes \mathsf{E})\frac{1}{z_2-v^2r(z_2)-H_0}\right].\end{aligned}$$

In general, the analysis of the dynamics is hampered by the intertwining of the integrals over z_1 and z_2. For the free toy model, the factor $1/(z_2-z_1)$ is now the only remaining coupling between the two contour integrals. We can eliminate this intertwining by first considering the time derivative of the reduced evolution,

$$\begin{aligned}\frac{d}{dt}\sigma(t) = &-\frac{v^2}{4\pi^2}\oint_\Gamma dz_1\, dz_2 e^{it(z_1-z_2)} \\ &(\mathbf{r}(z_1)-\mathbf{r}(z_2))\times \operatorname{Tr}\mathbb{E}\left[\frac{1}{z_1-v^2r(z_1)-H_0}(\sigma(0)\otimes \mathsf{E})\frac{1}{z_2-v^2r(z_2)-H_0}\right] \\ &-\frac{1}{4\pi^2}\frac{d}{dt}\oint_\Gamma dz_1\, dz_2 e^{it(z_1-z_2)}\mathbb{E}\left[\frac{1}{z_1-v^2r(z_1)-H_0}(\sigma(0)\otimes \mathsf{E})\frac{1}{z_2-v^2r(z_2)-H_0}\right].\end{aligned}$$

The Tr and $\mathbb{E}$ operations in this expression hide yet more integrals. If we look at the individual matrix elements of $\sigma(t)$, we can write out these operations as,

$$\begin{aligned}
\frac{d}{dt}\sigma_{ij}(t) &= -\frac{v^2}{4\pi^2}\sum_k \sigma_{kk}(0)\oint_\Gamma dz_1\, dz_2 e^{it(z_1-z_2)}\left(\mathbf{r}_{ij}(z_1)-\mathbf{r}_{ij}(z_2)\right)\\
&\times\int d\mu_E(x)\frac{1}{z_1-v^2r(z_1)-\epsilon_k-x}\frac{1}{z_2-v^2r(z_2)-\epsilon_k-x}\\
&-\frac{1}{4\pi^2}\sigma_{ij}(0)\frac{d}{dt}\oint_\Gamma dz_1\, dz_2 e^{it(z_1-z_2)}\\
&\times\int d\mu_E(x)\frac{1}{z_1-v^2r(z_1)-\epsilon_i-x}\frac{1}{z_2-v^2r(z_2)-\epsilon_j-x},
\end{aligned}$$

where we denote the probability density function of H_0^E under the initial environmental state as μ_E.

The most likely initial state of the environment is a Gibbs state, with a corresponding probability density function,

$$\mu_\beta = \begin{cases} \dfrac{\beta e^{-\beta x}}{2\sinh(h\beta)} & \text{if } -h<x<h,\\ 0 & \text{otherwise.}\end{cases}$$

Unfortunately, the resolvent mapping corresponding to this probability density function cannot be expressed in terms of simple algebraic functions. It can only be calculated numerically. In lack of a better understanding of the equilibrium resolvent mappings, we limit the further discussion of this two-level systems to initial states which correspond to energy eigenstates[12] .

For an initial state corresponding to an energy eigenstate of the Hamiltonian part H_0^E, the integration over x in the above equations falls away and we end up with a more manageable problem,

$$\begin{aligned}
\frac{d}{dt}\sigma_{ij}(t) &= -\frac{v^2}{4\pi^2}\sum_k \sigma_{kk}(0)\oint_\Gamma dz_1\, dz_2 e^{it(z_1-z_2)}\left(\mathbf{r}_{ij}(z_1)-\mathbf{r}_{ij}(z_2)\right)\\
&\times\frac{1}{z_1-v^2r(z_1)-\epsilon_k-x}\frac{1}{z_2-v^2r(z_2)-\epsilon_k-x}\\
&-\frac{1}{4\pi^2}\sigma_{ij}(0)\frac{d}{dt}\oint_\Gamma dz_1\, dz_2 e^{it(z_1-z_2)}\frac{1}{z_1-v^2r(z_1)-\epsilon_i-x}\frac{1}{z_2-v^2r(z_2)-\epsilon_j-x},
\end{aligned}$$

where now x is the energy of the environment in the initial state.

[12]The behavior of the system for equilibrium states can then be resolved by integrating with the measures μ_β over the solutions for initial energy states. This integration is numerically very complex and does not add any insights into the behavior of the system, so we do not discuss this.

Off-diagonal elements

For off-diagonal elements of the density matrix $\sigma(t)$ the above equation simplifies to,

$$\sigma_{ij}(t) = -\frac{1}{4\pi^2}\sigma_{ij}(0)\oint_{\Gamma} dz_1\, dz_2 e^{it(z_1-z_2)}\frac{1}{z_1 - v^2 r(z_1) - \epsilon_i - x}\frac{1}{z_2 - v^2 r(z_2) - \epsilon_j - x}.$$

The contour integrals in this equation are tantamount to performing a Fourier transform of the probability density function obtained by performing the limit,

$$\nu_x(u) = \lim_{w\to 0+}\frac{1}{2}\frac{1}{u + iw - v^2 r(u+iw) - \epsilon_i - x} - \frac{1}{u - iw - v^2 r(u-iw) - \epsilon_i - x}.$$

This limit can only be non-zero if u is on the support of the pdf associated to $\mathbf{r}_{ii}$. Furthermore, if both u and $x + \epsilon_i$ are on the interior of the support of this pdf, $\nu_x(u)$ is bounded. Only if $x + \epsilon_i$ and u are on the boundary of the support, can $\nu_x(u)$ become infinite. So, unless x corresponds to the energy in the ground state of the unperturbed environment, ν_x is an absolutely continuous, finite measure. The support of this measure cannot be larger than the support of the pdf associated to $\mathbf{r}_{ii}$. As such, $\nu_x(u)$ corresponds to an L^2-function and so its Fourier transform is again an L^2-function.

For $\sigma(t)$, this means that the off-diagonal elements will decay to zero for large times t. The decay rate depends on the specific form of the Hamiltonian. Figure 4.4 shows the generic behavior of $\sigma_{12}(t)$ under increasing coupling strength. Even in this very simple model, the behavior to equilibrium differs wildly depending on the interaction strength. For strong coupling, the decay is almost exponential, whereas for small coupling the decay creeps along according to some small power law.

Diagonal elements

The long-term behavior of the off-diagonal elements is not amenable to such an easy analysis as that of the off-diagonal elements. However, this behavior can be calculated quite easily numerically. We content ourselves here with showing a generic example of the time-evolution of the $(1,1)$-element of $\sigma(t)$ where $\sigma(0)$ corresponds to the $|0\rangle$-state.

4.5 Hamiltonian specter of amalgamated freely interacting systems

The first steps in the calculation of the reduced dynamics of a amalgamated free system can be stated for a more general situation than the model of section 4.1.3. In particular, the analogue of theorem 4.2 can be stated for *any* interaction term V which is free with amalgamation from H_0 over the system $\mathcal{S}$, not just for the more specific form (4.3).

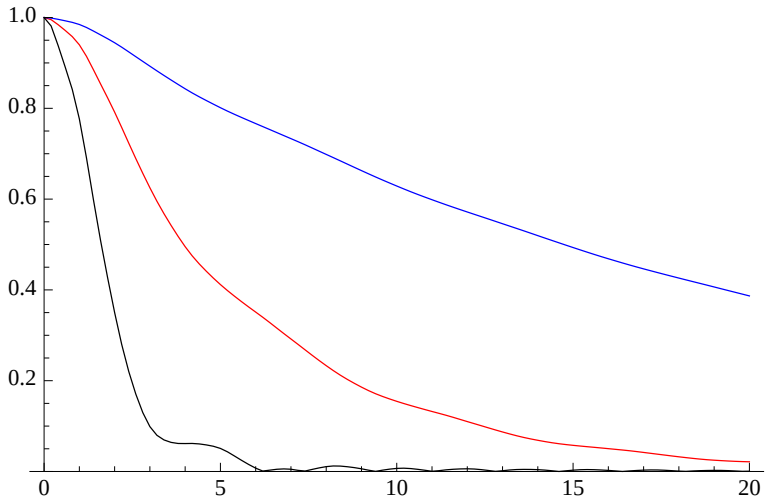


Figure 4.4: The decay of the absolute value of $\sigma_{12}(t)$ for increasing interaction strength. The three situations shown correspond, from top to bottom, to $v = 1/4$, $v = 1/2$ and $v = 1$.

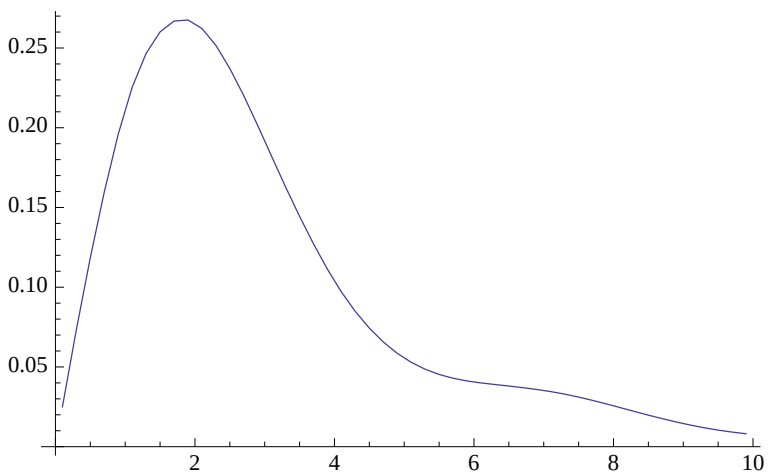


Figure 4.5: The figure shows the derivative of the $(1, 1)$-element of the reduced density matrix with respect to time for an interaction strength $v = 1$.

4.5.1 Another modified moment cumulant relation

As in the plain free case, we start our analysis of the amalgamated free system by modifying theorem 3.34 so that it retains the information about the operator structure of the unperturbed Hamiltonian.

The rescaling we used in section 4.3 is not required for the mathematics of this model. All calculations can be done directly using the conditionally expected resolvent mapping of the Hamiltonian H,

$$\mathbf{R}(z) = \mathbb{E}\left[\frac{1}{z - H}\right]. \tag{4.24}$$

Theorem 4.16. *Let H be a Hamiltonian in the algebra of a composite quantum system $\mathcal{S} \otimes \mathcal{E}$. Suppose that H can be written as $H_0 + V$, where H_0 is a non-interacting Hamiltonian and V is free with amalgamation from H_0 over $\mathcal{S}$ in the probability space $(\mathcal{S} \otimes \mathcal{E}, \mathbb{E})$. In a neighborhood of ∞, the conditionally expected resolvent $\mathbf{R}(z)$ is the unique solution of the self-consistent equation,*

$$\mathbf{R}(z) = \mathbb{E}\left[\frac{1}{z - K_V(\mathbf{R}(z)) - H_0}\right], \tag{4.25}$$

*where K_V is the $\mathcal{S}$-*valued *cumulant series of the interaction V.*

-

Proof. We can rewrite (4.24) in terms of the non-interacting Hamiltonian H_0 and the interaction term V,

$$\mathbf{R}(z) = \mathbb{E}\left[\frac{1}{z - H_0 - V}\right].$$

For sufficiently large $|z|$, the Neumann series,

$$N(z) := \sum_{n=0}^{\infty} (z - H_0)^{-1} \left(V(z - H_0)^{-1}\right)^n, \tag{4.26}$$

converges in norm to the resolvent mapping of H. Notice that it converges absolutely and we can thus rearrange terms in this series without perturbing the convergence. Equally important, all subseries converge, albeit to a different element in the algebra $\mathcal{S} \otimes \mathcal{E}$.

Existence of solutions

We begin by proving that if the Neumann series converges, it leads to the above equation. We can rewrite the expectation of (4.26) in terms of free cumulants,

where we use the shorthand $(z - H_0)^{-1} = A$ to compact the equations slightly,

$$n(z) := \mathbb{E}\left[N(z)\right] = \mathbb{E}\left[A\right] + \sum_{n=1}^{\infty} \mathbb{E}\left[A(VA)^n\right]$$
$$= \mathbb{E}\left[A\right] + \sum_{n=1}^{\infty} \sum_{\pi \in NC(2n)} k_\pi(A, \dot{V}, A, \underbrace{V, A, \ldots, V, A}_{(n-1) \text{ times}})$$

We can rearrange[13] the terms in the sum over $NC(2n)$ according to the number of elements connected by the bridge that starts at the dotted V; the first V which appears in the above expansion. Since A and V are free, the only non-zero cumulants are those which correspond to partitions where the bridges connect only A's or only V's or equivalently blocks with only even or only odd numbers.

For any n, there are exactly n V's, so the bridge that contains $\dot{V}$, connects at most n elements. If we denote the bridge which contains $\dot{V}$ by W_1,

$$n(z) = \mathbb{E}\left[A\right] + \sum_{n=1}^{\infty} \sum_{s=1}^{n} \sum_{\substack{W_1, \\ |W_1|=s, \\ 2 \in W_1}} \sum_{\substack{\pi = \{W_1, \ldots\} \\ \pi \in NC(2n+1)}} k_\pi(A, \dot{V}, A, V, A, \ldots, V, A) \qquad (4.27)$$

If $W_1 = (w_1 = 2, \ldots, w_s)$, then each remaining block W_k in $\pi = \{W_1, \ldots\}$ is wedged between some $w_{j(k)}$ and $w_{j(k)+1}$ on the circle, i.e.

$$\forall\, W_k \in \pi \,\text{and}\, k \neq 1, \exists!\, j(k) \in \{1, \ldots, 2n\} \looparrowright W_k \subset [w_{j(k)}, w_{j(k)+1}],$$

where $w_{s+1} := w_1$ and $[w_{j(k)}, w_{j(k)+1}]$ denotes an oriented circle segment. In other words, π can be decomposed as the union of s partitions σ_k and the bridge W_1,

$$\pi = \{W_1\} \cup \sigma_1 \cup \cdots \cup \sigma_s,$$

such that for all $k \leq s$, σ_k is a non-crossing partition of $\{w_k{+}1, w_k{+}2, \ldots, w_{k+1}{-}1\}$. As we stated before, the corresponding cumulant k_π, or in this case,

$$k_{\{\{W_1\} \cup \sigma_1 \cup \cdots \cup \sigma_s\}}(A, \dot{V}, A, \ldots, V, A)$$

is only non-zero if W_1 bridges only V's . For any k, this means that $\mathbb{1}_{[w_k+1, w_{k+1}-1]}$ corresponds to a bridge connecting all elements in the set

$$(\dot{A}, V, A, \ldots, V, \ddot{A}),$$

where $\dot{A}$ is the $(w_k + 1)^{th}$ element in the original word and $\ddot{A}$ the $(w_{k+1} - 1)^{th}$ element. The partition σ_s is a bit special, since in general it connects the first A in the original word to elements which are at the end of the original word. When

[13] This rearrangement does not alter the convergence properties of the Neumann series since we only permute terms under the sum over $NC(2n)$.

decomposing the cumulants in terms of the partition $\{W_1, \sigma_1, \dots, \sigma_s\}$, this simply means the outermost cumulant function is the one corresponding to σ_s.

$$k_\pi(A, \dot{V}, A, \underbrace{V, A \dots, V, A}_{(n-1)\text{ times}}) =$$

$$k_{\sigma_s}\Big(Ak_{W_1}\big(\dot{\hat{V}}, k_{\sigma_1}(A, \underbrace{V, A, \dots, V, A}_{\substack{(w_2-w_1-2)/2\\ \text{times}}})\hat{V}, \dots, k_{\sigma_{s-1}}(A, \underbrace{V, A, \dots, V, A}_{\substack{(w_{s-1}-w_{s-2}-2)/2\\ \text{times}}})\hat{V}\big), A, \underbrace{V, A, \dots, V, A}_{\substack{(2n-w_s)/2\\ \text{times}}}\Big),$$

where the V's with hats are those connected by W_1. If we plug this information into equation (4.27) we get

$$n(z) = \mathbb{E}[A] + \sum_{n=1}^{\infty}\sum_{s=1}^{n}\sum_{\substack{W_1,\\ |W_1|=s,\\ 2\in W_1}}\sum_{\substack{\pi=\{W_1,\dots\}\\ \pi\in NC(2n+1)}}$$

$$k_{\sigma_s}\Big(Ak_{W_1}\big(\dot{\hat{V}}, k_{\sigma_1}(A, \underbrace{V, A, \dots, V, A}_{\substack{(w_2-w_1-2)/2\\ \text{times}}})\hat{V}, \dots, k_{\sigma_{s-1}}(A, \underbrace{V, A, \dots, V, A}_{\substack{(w_{s-1}-w_{s-2}-2)/2\\ \text{times}}})\hat{V}\big), A, \underbrace{V, A, \dots, V, A}_{\substack{(2n-w_s)/2\\ \text{times}}}\Big).$$

The summation over W_1 is equivalent to a summation over a set $\{w_1, \dots, w_s\}$ if we demand that $2 = w_1 < \cdots < w_s \leq 2n$. The summation over π can then be replaced by a summation over all σ_k with appropriate conditions. We also rewrite k_{W_1} as k_s to signify that it only depends on W_1 through the number s and the arguments k_{σ_k}.

$$n(z) = \mathbb{E}[A] + \sum_{n=1}^{\infty}\sum_{s=1}^{n}\sum_{2=w_1<\cdots<w_s\leq 2n}\sum_{\sigma_k\in NC([w_k+1,w_{k+1}-1])}$$

$$k_{\sigma_s}\Big(Ak_s\big(\dot{\hat{V}}, k_{\sigma_1}(A, \underbrace{V, A, \dots, V, A}_{\substack{(w_2-w_1-2)/2\\ \text{times}}})\hat{V}, \dots, k_{\sigma_{s-1}}(A, \underbrace{V, A, \dots, V, A}_{\substack{(w_{s-1}-w_{s-2}-2)/2\\ \text{times}}})\hat{V}\big), A, \underbrace{V, A, \dots, V, A}_{\substack{(2n-w_s)/2\\ \text{times}}}\Big).$$

We change variables one last time and write $i_k := (w_{k+1} - w_k - 2)/2$ for $k < s$ and $i_s := (2n - w_s)/2$

$$= \mathbb{E}[A] + \sum_{n=1}^{\infty}\sum_{s=1}^{n}\sum_{\substack{i_1,\dots,i_s\in\\ \{0,\dots,n-1\}\\ i_1+\cdots+i_s=\\ n-s}}\sum_{\sigma_k\in NC(2i_k+1)}$$

$$k_{\sigma_s}\Big(Ak_s\big(\dot{\hat{V}}, k_{\sigma_1}(A, \underbrace{V, A, \dots, V, A}_{i_1\text{ times}})\hat{V}, \dots, k_{\sigma_{s-1}}(A, \underbrace{V, A, \dots, V, A}_{i_{s-1}\text{ times}})\hat{V}\big), A, \underbrace{V, A, \dots, V, A}_{i_s\text{ times}}\Big)$$

$$= \mathbb{E}[A] + \sum_{n=1}^{\infty} \sum_{\substack{i_1,\ldots,i_s \in \\ \{0,\ldots,n-1\} \\ i_1+\cdots+i_s = \\ n-s}}$$

$$\mathbb{E}\left[A \sum_{s=1}^{n} k_s \left(\dot{\hat{V}}, \mathbb{E}\left[A \underbrace{VA\cdots VA}_{i_1 \text{ times}} \right] \hat{V}, \ldots, \mathbb{E}\left[A \underbrace{VA\cdots VA}_{i_{s-1} \text{ times}} \right] \hat{V} \right) A \underbrace{VA\cdots VA}_{i_s \text{ times}} \right]$$

We now rearrange[14] all the terms in the summation, including terms corresponding to different values of n. We choose one index i_j and hold all other indices, as well as s, constant and collect all the terms corresponding to the different possible values of i_j. We then do the same for the other i_k's. After some sorting, we end up with

$$\begin{aligned} &= \mathbb{E}[A] + \mathbb{E}\left[A \sum_{s=1}^{\infty} k_s \left(\dot{\hat{V}}, \mathbb{E}\left[\frac{1}{z-H} \right] \hat{V}, \ldots, \mathbb{E}\left[\frac{1}{z-H} \right] \hat{V} \right) \frac{1}{z-H} \right] \\ &= \mathbb{E}[A] + \mathbb{E}\left[A\, K_V \left(\mathbb{E}\left[\frac{1}{z-H} \right] \right) \frac{1}{z-H} \right] \\ &= \mathbb{E}[A] + \mathbb{E}\left[A K_V\left(\mathbf{R}(z)\right) \frac{1}{z-H} \right]. \end{aligned} \tag{4.28}$$

We can reiterate the above calculation for the second term in (4.28) where the 'surplus' A which kept appearing at the front of each term is now replaced by $AK_V(\mathbf{R}(z))$. Doing this once, gives us

$$n(z) = \mathbb{E}[A] + \mathbb{E}\left[AK_V(\mathbf{R}(z))\right] + \mathbb{E}\left[AK_V(\mathbf{R}(z)) AK_V(\mathbf{R}(z)) \frac{1}{z-H} \right].$$

We can repeat this process an infinite amount of times, such that for sufficiently large $|z|$, it generates a convergent series and we obtain

$$n(z) = \sum_{n=0}^{\infty} \mathbb{E}\left[A \left(K_V\left(\mathbf{R}(z)\right) A \right)^n \right]. \tag{4.29}$$

Expression (4.29) is tantamount to equating two Neumann series which again for large enough $|z|$ converge to

$$\mathbf{R}(z) = \mathbb{E}\left[\frac{1}{z - H_0 - K_V\left(\mathbf{R}(z)\right)} \right]. \tag{4.30}$$

[14] This can be justified by recycling the argument in the proof of theorem 4.2. Although we are dealing with an operator-valued version here, the norm estimates stay essentially the same.

Uniqueness of solutions

The proof of theorem 4.2 can be recycled to prove uniqueness for the amalgamated free case as well. Consider first the formal definition of the operator-valued cumulant series of the random variable V.

$$K_V(b) = \sum_{n=1}^{\infty} k_n^{\mathbb{E}}(V, \underbrace{bV, \ldots, bV}_{(n-1)\text{ times}}), \quad \forall\, b \in \mathcal{S}.$$

For each of the terms $k_n^{\mathbb{E}}$ we have the estimate,

$$\|k_n^{\mathbb{E}}(V, bV, \ldots, bV)\| \leq 16^n \|V\|^n \, \|b\|^{n-1}.$$

This inequality implies that at least if $b \leq (16\|V\|)^{-1}$, the cumulant series converges in norm to some bounded operator on $\mathcal{S}$.

The second ingredient needed to continue the argument,is holomorphy of the map K_V, when viewed as a operator-valued map on the domain $\mathcal{D} = \{w \,|\, w \in \mathcal{S} \,\&\, \|w\| \leq (16\|V\|)^{-1}\}$. As a concatenation of sums and products of holomorphic maps, K_V is holomorphic whenever it converges, so in particular on $\mathcal{D}$.

With that in mind, we can define a map F_z on $\mathcal{D}$ as,

$$F_z(w) = \mathbb{E}\left[\frac{1}{z - K_V(w) - H_0}\right],$$

which for sufficiently large $|z|$ is bounded and holomorphic and maps $\mathcal{D}$ strictly to its interior. According to the Earle-Hamilton theorem, F_z is then a strict contraction in the Carathéodory metric and we are guaranteed that on this domain our equations produce a unique solution. Moreover, this domain is compatible with the domain where the constructive part of our proof holds. So, the unique solution of the above fixed point equation is $\mathbf{R}(z)$.

□

The formal equivalence between the proofs of theorem 4.2 and theorem 4.16 allows us to simply copy most of the remarks made in section 4.3.1 to the amalgamated free case.

Holomorphic extensions

Analogous to theorem 4.6, we can extend the validity of theorem 4.16 to a more sensible domain $\mathcal{F} = \{z \,|\, |\mathrm{Im}\ z| > 6\|V\|\}$.

Theorem 4.17. *Let H be a Hamiltonian in the algebra of a composite quantum system $\mathcal{S} \otimes \mathcal{E}$. Suppose that H can be written as $H_0 + V$, where H_0 is a non-interacting Hamiltonian and V is free with amalgamation from H_0 over $\mathcal{S}$ in the*

probability space $(\mathcal{S} \otimes \mathcal{E}, \mathbb{E})$. ~~*In a neighborhood of* ∞~~ *The conditionally expected resolvent* $\mathbf{R}(z)$ *is the unique solution of the self-consistent equation,*

$$\mathbf{R}(z) = \mathbb{E}\left[\frac{1}{z - K_V(\mathbf{R}(z)) - H_0}\right], \quad \forall\, z \text{ s.t. } |Im\ z| > 6\|V\|, \tag{4.31}$$

where K_V *is the* $\mathcal{S}$*-valued cumulant series of the interaction* V*.*

-

Proof. The proof of this theorem is completely analogous to the proof of theorem 4.6.

□

Solution strategy

The solution strategy for the self-consistent equation (4.25) remains the same as in the plain free case. Repeated application of the map F_z

$$F_z(w) := \mathbb{E}\left[\frac{1}{z - K_V(w) - H_0}\right], \quad \forall\, z \in \mathcal{F},\ w \in \mathcal{D}, \tag{4.32}$$

drives the result to the unique fixed point of F_z which is the expected resolvent $\mathbf{R}(z)$. This follows immediately from theorem 4.17.

The technical implementation of this algorithm is slightly more complicated than in the plain free case. The fixed point equation (4.32) is now a full matricial equation which cannot be reduced a set of scalar equations which hold for all z. As a result, the solving time no longer scales linearly with the size of the system S, but goes up with the cube of the system size. Although for larger systems, this can present a major problem, a cubic scaling is the smallest possible non-trivial scaling for generic quantum dynamical systems and a substantial improvement over the original problem.

Model-specific features

Recall that for the amalgamated free model, the interaction is of the form

$$V = \sum_{i \leq j}^{d} F_{ij} \otimes V_{ij}.$$

The additional structure of the interaction term allows us to reduce the complexity of the problem somewhat. For any element $w \in \mathcal{S}$, the $\mathcal{S}$-valued cumulant series of

V reduces to,

$$\begin{aligned} K_V^{\mathbb{E}}(w) &= \sum_{s=1}^{\infty} \sum_{i \leq j}^{d} k_s^{\mathbb{E}} \left((F_{ij} \otimes V_{ij}), w(F_{ij} \otimes V_{ij}), \cdots, w(F_{ij} \otimes V_{ij}) \right) \\ &= \sum_{s=1}^{\infty} \sum_{i \leq j}^{d} k_s^{\mathbb{E}} \left(\mathbb{1} \otimes V_{ij}, F_{ij} w \otimes V_{ij}, \cdots, F_{ij} w \otimes V_{ij} \right) F_{ij} \\ &= \sum_{s=1}^{\infty} \sum_{i \leq j} k_s^{\tau\mathcal{E}} \left(V_{ij}, \cdots, V_{ij} \right) \left(F_{ij}\, w \right)^{s-1} F_{ij} \\ &:= \sum_{i \leq j}^{d} K_{V_{ij}}^{\tau\mathcal{E}} \left(F_{ij} w \right) F_{ij}, \end{aligned} \tag{4.33}$$

where we have defined $K_V^{\tau\mathcal{E}}$ on $\mathcal{S}$ through the holomorphic functional calculus.

This makes the analysis of the fixed point equation a bit more straightforward. The rather awkward definition of the full operator-valued cumulant series is now reduced to calculating the scalar-valued functions $K_{V_{ij}}^{\tau\mathcal{E}}(z)$ on $\mathbb{C}$ and extending them to functions on $\mathcal{S}$ through the holomorphic functional calculus[15].

The complexity class of the problem is not altered by this additional structure. The running time of the fixed point algorithm still scales with the cube of the system size in general.

The reduced form (4.33) does make it easier to detect situations where better scalings can be obtained, i.e. when the global system has additional symmetries. We will illustrate this in the analysis of our amalgamated free toy model.

4.5.2 An amalgamated free toy model specter

The formal equivalence between theorem 4.2 and theorem 4.16 does not extend to an equivalence between the behavior of the models of section 4.1.2 and section 4.1.3. In this section, we illustrate this difference by applying theorem 4.16 to the amalgamated free toy model of section 4.2.

Recall that in our qubit toy model, the interaction V is assumed to be an operator-valued semicircular element of the form

$$V = \begin{pmatrix} a & b \\ b & c \end{pmatrix}, \quad V \in \mathcal{M}_2(\mathcal{E}),$$

where $\{a, b, c\}$ is a free family of semicircular elements in the probability space $(\mathcal{E}, \tau_{\mathcal{E}})$, each with their own mean m_i and variance v_i.

[15] Note that we cannot define the function $K_{V_{ij}}^{\tau\mathcal{E}}$ on $\mathcal{S}$ through the continuous functional calculus, which is only defined for normal operators. Elements of $\mathcal{S}$ and in particular the arguments $w\, F_{ij}$ need not be normal.

For such a semicircular element, the cumulant series can be calculated directly using the basic definition of cumulant series or alternatively using equation (4.33). We will handle the latter case.

In the probability space $(\mathcal{E}, \tau_{\mathcal{E}})$, the cumulant series of the random variables a, b and c are all affine maps of the form,

$$\begin{aligned} k_a^{\tau\varepsilon}(z) &= m_a + v_a^2 z, \\ k_b^{\tau\varepsilon}(z) &= m_b + v_b^2 z, \\ k_c^{\tau\varepsilon}(z) &= m_c + v_c^2 z. \end{aligned}$$

They can be extended to holomorphic maps on $\mathcal{S}$ through the holomorphic functional calculus. Since the above maps are all affine, this extension is almost trivial,

$$\begin{aligned} K_a^{\mathbb{E}}(w) &= m_a \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + v_a^2 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \\ K_b^{\mathbb{E}}(w) &= m_b \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + v_b^2 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\ K_c^{\mathbb{E}}(w) &= m_c \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + v_c^2 \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \end{aligned}$$

The trio $K_a^{\mathbb{E}}$, $K_b^{\mathbb{E}}$ and $K_c^{\mathbb{E}}$ preserves the positivity of the anti-Hermitian part of w and are all three holomorphic on $\mathcal{S}$. The map $K_V^{\mathbb{E}} = K_a^{\mathbb{E}} + K_b^{\mathbb{E}} + K_c^{\mathbb{E}}$ thus extends to a, not only holomorphic, but also Herglotz map on $\mathcal{S}^+ \cup \mathcal{S}^-$. The validity of the fixed point equation then extends to the entire space $\mathcal{S}^+ \cup \mathcal{S}^-$. For any $z \in \mathbb{C}\backslash\mathbb{R}$, $\mathbf{R}(z)$ is the unique solution of the fixed point equation,

$$\mathbf{R}(z) = \mathbb{E}\left[\left(z - K_V(\mathbf{R}(z)) - \begin{pmatrix} \epsilon + H_0^E & 0 \\ 0 & -\epsilon + H_0^E \end{pmatrix}\right)^{-1}\right].$$

Remark 4.18 (Pastur equations)**.** In that case that $m_a = m_b = m_c = 0$ and also v_a and v_c are zero, these equations are known as Pastur's equations. These equations were first derived in [10] by Pastur and Lebowitz by a thermodynamic limit of a random GUE matrix interaction model. As such, this specific case of our amalgamated free toy model is equivalent to the case presented in [10], as the amalgamated freeness of the interaction V is easily seen to arise in the thermodynamic limit of the matrix interactions of [10].

-

4.6 Dynamics of amalgamated freely interacting systems

The amalgamated free model doesn't lend itself very well to a description in terms of a single dynamical equation in the spirit of theorem 4.14. It is more convenient

to first calculate the two point function $\mathbf{R}(z_1, z_2)$,

$$\mathbf{R}(z_1, z_2) := \mathbb{E}\left[\frac{1}{z_1 - H}\sigma(0) \otimes \mathsf{E}\frac{1}{z_2 - H}\right],$$

to a sufficient numerical precision on a predetermined curve γ which circles the spectrum of H. The time-dependent density matrix $\sigma(t)$ can then be calculated from this two-point function as

$$\sigma(t) = -\frac{1}{4\pi^2}\oint_{\Gamma} dz_1 dz_2\, e^{it(z_1 - z_2)}\, \mathbf{R}(z_1, z_2).$$

As in the plain free case, we start the analysis with a lemma which connects the two-point function $\mathbf{R}(z_1, z_2)$, to the expected resolvent $\mathbf{R}(z)$.

Lemma 4.19. *Let H be the Hamiltonian of a composite quantum system $S + E$. Suppose that H can be written as $H_0 + V$, where H_0 is a non-interacting Hamiltonian and V is free with amalgamation from H_0 over $\mathcal{S}$ in the probability space $(\mathcal{S} \otimes \mathcal{E}, \mathbb{E})$. If $|Im\ z_1| > 6\|V\|$ and $|Im\ z_2| > 6\|V\|$, the two point function $\mathbf{R}(z_1, z_2)$,*

$$\mathbf{R}(z_1, z_2) = \mathbb{E}\left[\frac{1}{z_1 - H}\sigma(0) \otimes \mathsf{E}\frac{1}{z_2 - H}\right], \tag{4.34}$$

is amenable to a description in terms of the conditionally expected resolvent mapping of H,

$$\begin{aligned}\mathbf{R}(z_1, z_2) =& \mathbb{E}\left[\frac{1}{z_1 - K_V(\mathbf{R}(z_1)) - H_0}(\sigma(0) \otimes \mathsf{E})\frac{1}{z_2 - K_V(\mathbf{R}(z_2)) - H_0}\right] \\ &+ \mathbb{E}\left[\frac{1}{z_1 - K_V(\mathbf{R}(z_1)) - H_0}\mathbf{L}(\mathbf{R}(z_1, z_2))\frac{1}{z_2 - K_V(\mathbf{R}(z_2)) - H_0}\right],\end{aligned} \tag{4.35}$$

where $\mathbf{L} : \mathcal{S} \to \mathcal{S}$ is the map,

$$\mathbf{L} := \sum_{s,t=1}^{\infty} k_{s+t}\left(V, \mathbf{R}(z_1)V, \ldots, \mathbf{R}(z_1)V, \mathbf{R}(z_1, z_2)V, \mathbf{R}(z_2)V, \ldots, \mathbf{R}(z_2)V\right).$$

-

Proof. We have relegated the proof of this lemma to the appendix. It can be found in section B.3.

□

In contrast to linear relation in the plain free case, the resulting expression for the two-point function $\mathbf{R}(z_1, z_2)$ is a hugely complicated self-consistent affine equation. What makes equation (4.35) so complicated, is the appearance of the full operator-valued cumulant series of V under the guise of the map $\mathbf{L}$. As we

have remarked more than once in chapter 3, the distribution and so by extension also the cumulant series, of a general operator is a very information-rich structure. Even if we merely want to write out explicitly the effect of the map $\mathbf{L}$, we not only need to specify the spectral measure of V, but also how it interact with each and every operator in $\mathcal{S}$.

It is highly implausible that an observer of the system $\mathcal{S}$ has access to sufficient information to characterize the most general forms of such a cumulant series. Up until now, such considerations were not important, since we could just as easily handle the general case as the more restrictive model of section 4.1.3. The complexity of lemma 4.19 changes this. Without the restrictions[16] of section 4.1.3, the relation (4.35) in the above lemma would mean a dead end for the analysis of amalgamated free interactions.

Model-specific features

Recall from section 4.1.3, that in the amalgamated free model the interaction V is of the form,

$$V = \sum_{i \leq j} F_{ij} \otimes V_{ij},$$

such that V is Hermitian and the V_{ij} form a free family of Hermitian operators in the probability space $(\mathcal{E}, \tau_{\mathcal{E}})$.

In section 4.5 we derived an alternative construction method for the cumulant series of V. We can now use a similar method to rewrite the map $\mathbf{L}$ in a more convenient format.

$$\begin{aligned}
\mathbf{L} &= \sum_{s,t}^{\infty} k_{s+t}^{\mathbb{E}}\left(V, \mathbf{R}(z_1)V, \ldots, \mathbf{R}(z_1)V, \mathbf{R}(z_1,z_2)V, \mathbf{R}(z_2)V, \ldots, \mathbf{R}(z_2)V\right) \\
&= \sum_{i \leq j} \sum_{s,t} k_{s+t}^{\mathbb{E}}\big(\mathbb{1} \otimes V_{ij}, F_{ij}\mathbf{R}(z_1) \otimes V_{ij}, \ldots, F_{ij}\mathbf{R}(z_1) \otimes V_{ij}, \\
&\qquad F_{ij}\mathbf{R}(z_1,z_2)F_{ij} \otimes V_{ij}, \mathbf{R}(z_2)F_{ij} \otimes V_{ij}, \ldots, \mathbf{R}(z_2)F_{ij}\big) \\
&= \sum_{i \leq j} \sum_{s,t} k_{s+t}^{\tau_{\mathcal{E}}}(V_{ij}, \ldots, V_{ij})\big(F_{ij}\mathbf{R}(z_1)\big)^{s-1}\Big(F_{ij}\mathbf{R}(z_1,z_2)F_{ij}\Big)\big(\mathbf{R}(z_2)F_{ij}\big)^{t-1}.
\end{aligned}$$

Although the resulting expression for the map $\mathbf{L}$ is still rather complicated, is shows more clearly the true nature of the self-consistent equation of lemma 4.19. The map $\mathbf{L}$,

$$\mathbf{L}(w, z_1, z_2) = \sum_{i \leq j} \sum_{s,t} k_{s+t}^{\tau_{\mathcal{E}}}(V_{ij}, \ldots, V_{ij})\big(F_{ij}\mathbf{R}(z_1)\big)^{s-1}\Big(F_{ij}wF_{ij}\Big)\big(\mathbf{R}(z_2)F_{ij}\big)^{t-1}, \tag{4.36}$$

[16] It is possible to dream up a different set of restrictions such that we can also continue the analysis, though we have not analyzed any such alternatives.

is linear in the argument w. The full expression of (4.35) is thus an affine equation with a unique fixed point, $\mathbf{R}(z_1, z_2)$. This fixed point can be calculated in the same manner as fixed points of ordinary affine equations on vector spaces can be calculated. As an example, we provide some details on the amalgamated free toy model.

4.6.1 Dynamical behavior of a two-level system

For our toy model, lemma 4.19 reduces to,

Lemma 4.20. *Let H be a Hamiltonian of a dynamical model as proposed in section 4.2. On $\mathbb{C}\backslash\mathbb{R}$, the two point function $\mathbf{R}(z_1, z_2)$,*

$$\mathbf{R}(z_1, z_2) = \mathbb{E}\left[\frac{1}{z_1 - H}\sigma(0) \otimes \mathsf{E}\frac{1}{z_2 - H}\right],$$

is amenable to a description in terms of the conditionally expected resolvent mapping of H,

$$\begin{aligned}\mathbf{R}(z_1, z_2) = &\mathbb{E}\left[\frac{1}{z_1 - K_V(\mathbf{R}(z_1)) - H_0}(\sigma(0) \otimes \mathsf{E})\frac{1}{z_2 - K_V(\mathbf{R}(z_2)) - H_0}\right] \\ &+ \mathbb{E}\left[\frac{1}{z_1 - K_V(\mathbf{R}(z_1)) - H_0}\mathbf{L}(\mathbf{R}(z_1, z_2))\frac{1}{z_2 - K_V(\mathbf{R}(z_2)) - H_0}\right],\end{aligned}$$

where $\mathbf{L}$ is the map,

$$\mathbf{L} = K_V(\mathbf{R}(z_1, z_2)) = \mathbb{E}\left[V\mathbf{R}(z_1, z_2)V\right] - \mathbb{E}\left[V\right]\mathbf{R}(z_1, z_2)\mathbb{E}\left[V\right].$$

-

In light of the remark made at the end of section 4.5.2, we limit the further discussion to a parameter range consistent with Pastur's model, i.e. $m_a = m_b = m_c = v_a = v_c = 0$. For Pastur's model, the fixed-point equation of theorem 4.16 reduces to

$$\mathbf{R}(z) = \mathbb{E}\left[\left(z - v_b^2\begin{pmatrix}\mathbf{R}_{22}(z) & \mathbf{R}_{21}(z)\\ \mathbf{R}_{12}(z) & \mathbf{R}_{11}(z)\end{pmatrix} - \begin{pmatrix}\epsilon + H_0^E & 0\\ 0 & -\epsilon + H_0^E\end{pmatrix}\right)^{-1}\right].$$

As remarked in section 4.5.2, the diagonal matrices form an invariant subalgebra for this fixed-point equation. In our search for fixed-points, we can thus restrict ourselves to diagonal $\mathbf{R}(z)$. This allows us also to rewrite the previous matricial equation as a set of two scalar equations,

$$\begin{cases}\mathbf{R}_{11}(z) = \tau\left[\left(z - v_b^2\,\mathbf{R}_{22}(z) - \epsilon - H_0^E\right)^{-1}\right],\\ \mathbf{R}_{22}(z) = \tau\left[\left(z - v_b^2\,\mathbf{R}_{11}(z) + \epsilon - H_0^E\right)^{-1}\right],\end{cases}$$

and we can choose $\mathbf{R}_{12}(z)$ and $\mathbf{R}_{21}(z)$ identically zero.

As $\mathbf{R}(z)$ is, for any z, a diagonal matrix, the equations of lemma 4.20 can also be rewritten succinctly in a scalar form.

$$\begin{aligned}
&\mathbf{R}_{ij}(z_1, z_2) = \\
&\sigma_{ij}(0)\, \tau_{\mathcal{E}} \left[\frac{1}{z_1 - v_b^2\, \mathbf{R}_{ii}(z_1) + (-1)^i \epsilon - H_0^E}\, \mathsf{E}(H_0^E)\, \frac{1}{z_2 - v_b^2\, \mathbf{R}_{jj}(z_2) + (-1)^j - H_0^E} \right] \\
&+ v_b^2\, (F \mathbf{R}(z_1, z_2) F)_{ij}\, \tau_{\mathcal{E}} \left[\frac{1}{z_1 - v_b^2\, \mathbf{R}_{ii}(z_1) + (-1)^i \epsilon - H_0^E}\, \frac{1}{z_2 - v_b^2\, \mathbf{R}_{jj}(z_2) + (-1)^j - H_0^E} \right].
\end{aligned}$$

These equations are very reminiscent of the equations governing the dynamics of the plain free toy model. The remaining analysis up to the dynamical behavior of this system is completely analogous to the plain free model.

4.7 Discussion

In many situations, a description of a quantum system as an isolated system is untenable. Even on very small timescales and under ideal laboratory conditions, a quantum system under study will interact with various degrees of freedom associated to the environment. It is therefore necessary to include the environment in the description of the system under study.

A full microscopic description of both system and environment is often impossible for two reasons. 1. The Hamiltonian governing the environment and the interaction terms coupling the system to its environment are rarely known. 2. Even if the full Hamiltonian governing system and environment is known, the resulting dynamics may be too complicated to analyze as such situations very rarely lead to integrable models.

The key to succes for any reduced description is to provide just the right amount of information on the system and more importantly its environment. If we provide too little information, the resulting description will not correspond in sufficient detail to the actual dynamics. If we provide too much information, the reduced description resolves more detail, but also becomes harder to construct and analyze.

In this chapter, we constructed and discussed a novel reduced description based on free random variables. We made a single assumption on the nature of the interaction between the system and its environment, namely that in good approximation the interaction can be modelled as a unitarily invariant random matrix. We have heuristically argued why such random matrices might be thought of as generic interactions. Moreover, such random matrices have been shown to model in good approximation chaotic and disordered quantum systems.

In the limit of infinite-size matrices, unitarily invariant random matrices converge to free random variables. In this limit, the randomness effectively freezes and mixed moments of both the interaction terms and the unperturbed Hamiltonian

become deterministic. Mixed moments are then completely determined by the spectral measures of the unperturbed Hamiltonian and the interaction terms. Much of the physically accessible information about the system and its environment is encoded in these spectral measures. If we assume that an observer only has access to macroscopic information about the environment, than most likely any and all such macroscopic observables commute. Ergo, it is possible to construct a single scalar measure which encodes all the information obtained by measurements of these observables. If the environment is much larger than the system under study, this constructed measure should be in good agreement with the spectral measure of the environmental part of the unperturbed Hamiltonian. The assumption of freeness thus allows us to input any and all physical information we have about an environment in the model.

The second critical part of any useful reduced description is that the dynamics is actually computable. Although admittedly a free interaction model is more complicated than say a Markovian approximation, the resulting dynamics can still be solved quite efficiently. The added computation complexity also allows us to resolve aspects of the dynamics which cannot be part of any Markovian approximation. In particular, the free interactions induce memory effects in the dynamics.

APPENDIX A

Numerical recipes for freely interacting systems

In chapter 3 it was explained how free random variables in a probability space $(\mathcal{A}, \varphi)$ can be canonically thought of as operators on an appropriate full Fock space. It is important to remark that in this scheme the full Fock space picture is not tied to a *representation* of the algebra $\mathcal{A}$. Specifically, in going over to the full Fock space picture, the Hermitian conjugate operation loses its meaning. For a general self-adjoint operator a in the algebra $\mathcal{A}$, the corresponding operator $F(a)$ on the degenerate full Fock space is no longer Hermitian. Although mathematicians probably do not overly care about this, a physicist cannot accept such a framework as a tool for his or her intuition. Moreover, the full Fock space picture of chapter 3 is not very well suited for numerical approximations of the free convolution or of solutions of the self-consistent equation in theorem 4.2.

In this section we develop a more physical picture based on so-called *interacting Fock spaces* which also allows for a straightforward method to approximate numerically the free convolution of two random operators.

A.1 Interacting Fock spaces

Consider a probability space $(\mathcal{A}, \varphi)$ over $\mathbb{C}$ where $\mathcal{A}$ is generated by a single random variable a. The algebra $\mathcal{A}$ can be canonically represented on a separable Hilbert space $\mathcal{H}$ via the GNS-construction for the state φ. This construction provides a representation π and a cyclic vector Ω such that

$$\varphi(a) = \langle \Omega | \pi(a) | \Omega \rangle, \qquad \forall a \in \mathcal{A}, \tag{A.1}$$

and

$$\overline{\mathrm{Span}\Big(\{\pi(a)|\Omega\rangle \,|\, a \in \mathcal{A}\}\Big)} = \mathcal{H} \simeq \mathcal{L}^2\left(\sigma(a), \mu_a\right). \tag{A.2}$$

Typically, the GNS-construction would be used to represent the operator a as a multiplication operator on $\mathcal{L}^2\left(\sigma(a), \mu_a\right)$. From a numerical point of view though, it is preferable to represent a as a Jacobi matrix[1] on an ℓ_2-space. The easiest way to see how these different representations are related, is to explicitly construct the isomorphisms involved.

A basis for the GNS representation

Let us first see how we can construct an isomorphism between $\mathcal{H}$ and $\mathcal{L}^2\left(\sigma(a), \mu_a\right)$. From the spectral theorem, we know that for any bounded, continuous function f, the expectation value $\varphi\left(f(a)\right)$ can be rewritten as an integral over the spectrum of a,

$$\varphi\left(f(a)\right) = \int\limits_{\sigma(a)} f(x)\, \mu_a(dx). \tag{A.3}$$

Such a function f can be identified with an element of $\mathcal{L}^2\left(\sigma(a), \mu_a\right)$ if

$$\int\limits_{\sigma(a)} f(x)^2\, \mu_a(dx) < \infty, \tag{A.4}$$

which is equivalent to the requirement that $\varphi\left(f(a)^2\right) < \infty$. Since, by assumption, a is a bounded operator, all moments $\varphi(a^{2n})$ exist:

$$\varphi(a^{2n}) = \int\limits_{\sigma(a)} (x^n)^2 \mu_a(dx) < \infty, \quad \forall n \in \mathbb{N}, \tag{A.5}$$

and so for any $n \in \mathbb{N}$, the functions $f : x \mapsto x^n$ are $\mathcal{L}^2$-functions. Together, they generate a dense subset of $\mathcal{L}^2\left(\sigma(a), \mu_a\right)$. By applying the Gram-Schmidt procedure to the set $\{1, x, x^2, \ldots\}$ (in that order), we can construct a generating orthogonal set[2] $(P_i(x))_i$ for $\mathcal{L}^2\left(\sigma(a), \mu_a\right)$,

$$P_0(x) = 1, \tag{A.6}$$

$$P_1(x) = x - \int x P_0(x)\, \mu_a(dx), \tag{A.7}$$

$$P_2(x) = x^2 - P_1(x) \int x^2 P_1(x)\, \mu_a(dx) - P_0(x) \int x^2 P_0(x)\, \mu_a(dx), \tag{A.8}$$

$$\ldots \tag{A.9}$$

[1] A Jacobi matrix is a real, symmetric tridiagonal matrix with bounded positive off-diagonal elements.

[2] The $P_i(x)$ are of course the classical orthogonal polynomials associated to the measure μ_a and as such have some very nice properties which we will use later on.

By normalizing this set, we end up with a basis $(p_i(x))_i$ for $\mathcal{L}^2(\sigma(a), \mu_a)$. By virtue of the Gram-Schmidt procedure, $p_k(x)$ is orthogonal to any polynomial of an order lower than k. We can utilize this knowledge to determine a three term recurrence relation:

$$\alpha_{n+1}p_{n+1}(x) = (x - \beta_{n+1})p_n(x) - \alpha_n p_{n-1}(x), \tag{A.10}$$

where the coefficients α_n and β_n are determined by the measure μ_a,

$$\alpha_n = \int x\, p_{n-1}(x)\, p_n(x)\mu_a(dx), \tag{A.11}$$

$$\beta_{n+1} = \int x\, p_n(x)\, p_n(x)\mu_a(dx). \tag{A.12}$$

Remark that due to the Gram-Schmidt procedure, in any $p_k(x)$ the coefficient h_k of the highest power of x is always positive and h_k/h_{k+1} is equal to α_n, so clearly the α_n are also strictly positive.

Through the spectral theorem, the basis $(p_i(x))_i$ has a canonical counterpart $(e_i)_i$ in $\mathcal{H}$,

$$\begin{aligned}
\delta_{i,j} &= \int p_i(x)p_j(x)\mu(dx) && \text{(A.13)}\\
&= \varphi(p_i(a)p_j(a)) && \text{(A.14)}\\
&= \langle\Omega|\pi(p_i(a)p_j(a))|\Omega\rangle && \text{(A.15)}\\
&= \langle\Omega\, p_i(a)\,|\, p_j(a)\Omega\rangle && \text{(A.16)}\\
&= \langle e_i\,|\, e_j\rangle, && \text{(A.17)}
\end{aligned}$$

if we make the identification $\pi(p_i(a))|\Omega\rangle = |e_i\rangle$. The operation $U : p_i(x) \mapsto e_i$ then extends to the desired isomorphism between $\mathcal{H}$ and $\mathcal{L}^2(\sigma(a), \mu_a)$. The isomorphism between $\mathcal{H}$ and $\ell_2(\mathbb{N})$ extends from the trivial identification of e_i with the vector $(\delta_{i,j})_j \in \ell_2(\mathbb{N})$, which we will also denote f_i.

Jacobi matrix representation of a random variable

Using the basis $(e_i)_i$ and the above isomorphisms, we can represent the random variable a as a operator on ℓ_2,

$$A := \pi_{\ell_2}(a) = \sum_{i,j\in\mathbb{N}} \langle e_i|\pi_{\mathcal{H}}(a)|e_j\rangle |f_j\rangle\langle f_i|, \tag{A.18}$$

where

$$\begin{aligned}
\langle e_i|\pi_{\mathcal{H}}(a)|e_j\rangle &= \int p_i(x)\, x\, p_j(x)\mu_a(dx) && \text{(A.19)}\\
&= \int p_i(x)\Big(\alpha_{j+1}p_{j+1}(x) + \beta_{j+1}p_j(x) + \alpha_j p_{j-1}\Big)\mu_a(dx) && \text{(A.20)}\\
&= \delta_{i,j+1}\alpha_i + \delta_{i,j}\beta_{j+1} + \delta_{i,j-1}\alpha_j. && \text{(A.21)}
\end{aligned}$$

So, because of the particular nature of our basis vectors, A reduces to an (infinite-dimensional) tridiagonal symmetric matrix with positive off-diagonal elements.

$$A = \begin{pmatrix} \beta_1 & \alpha_1 & & & 0 \\ \alpha_1 & \beta_2 & \alpha_2 & & \\ & \alpha_2 & \beta_3 & \ddots & \\ & & \ddots & \ddots & \\ 0 & & & & \end{pmatrix}. \tag{A.22}$$

Any matrix with the above properties is called a *Jacobi marix*. Jacobi matrices are very useful tools in studying absolutely continuous measures since they allow for some easy and fast numerical approximation schemes that can be efficiently implemented in computer algorithms.

Numerical approximation of absolutely continuous measures

If we denote by A_n the truncation of A to $M_n(\mathbb{C})$, then

$$A_n = \begin{pmatrix} \beta_1 & \alpha_1 & & & 0 \\ \alpha_1 & \beta_2 & \alpha_2 & & \\ & \alpha_2 & \beta_3 & \ddots & \\ & & \ddots & \ddots & \alpha_n \\ 0 & & & \alpha_n & \beta_n \end{pmatrix}. \tag{A.23}$$

Such a truncation is again a tridiagonal symmetric matrix with positive off-diagonal entries, but no longer infinite-dimensional. Its expected resolvent mapping $\langle\Omega|(z - A_n)^{-1}|\Omega\rangle$ is however again a twisted Herglotz function and we can interpret this function as the Cauchy transform of a now discrete measure on the real line. Up to order n, the moments of A_n are exactly the moments of the original matrix A,

$$\langle\Omega|A^k|\Omega\rangle = \langle\Omega|A_n^k|\Omega\rangle, \qquad \forall k \leq n. \tag{A.24}$$

Furthermore, since A_n can be derived from A by a compression, the eigenvalues of A_n interlace those of A, i.e. any eigenvalue λ_n of A_n is wedged between two eigenvalues κ and ν of A.

From this, it should be clear that the measures of A_n's converge in distribution to the measure of A and $\operatorname{supp}\mu_{A_n} \subset \operatorname{supp}\mu_A$. Using the boost group, we can even proof that this convergence will be exponentially fast in the ℓ_2-norm.

The GNS representation as an interacting Fock space

We can decompose the matrix A (and also any A_n) as a sum of a diagonal matrix and weighted shift operators,

$$A = S_A + D_A + S_A^*, \tag{A.25}$$

where

$$S_A = \begin{pmatrix} 0 & \alpha_1 & & & 0 \\ & 0 & \alpha_2 & & \\ & & 0 & \ddots & \\ & & & \ddots & \\ 0 & & & & \end{pmatrix}, \quad D_A = \begin{pmatrix} \beta_1 & 0 & & & 0 \\ 0 & \beta_2 & 0 & & \\ & 0 & \beta_3 & \ddots & \\ & & \ddots & \ddots & \\ 0 & & & & \end{pmatrix}. \tag{A.26}$$

(A.27)

The operators S_A and S_A^* act as weighted annihilation and creation operators on the basis of the GNS-space $\mathcal{H}$,

$$S_A^* |e_i\rangle = \alpha_{i+1} |e_{i+1}\rangle, \tag{A.28}$$
$$S_A |e_i\rangle = \alpha_{i-1} |e_{i-1}\rangle. \tag{A.29}$$

As a pair, they generate the entire Hilbert space $\mathcal{H}$ by application to the vacuum vector Ω. In reference to how the full and symmetric Fock spaces are constructed, from now on we refer to the GNS-representation space as an *interacting Fock space*. For future reference, an isomorphism between this interacting Fock space and the Full Fock space can be constructed from the formal identification of basis vectors

$$|\Omega\rangle \sim |\Omega\rangle \tag{A.30}$$
$$|e_i\rangle \sim |\otimes^i h\rangle, \tag{A.31}$$

where h is the normalized vector in a one-dimensional Hilbert space K. The full Fock space constructed from this Hilbert space, is then $\mathcal{F}(\mathcal{K})$.

A.2 Free products of interacting Fock spaces

A natural question at the end of the previous section is whether the concept of interacting Fock spaces can be extended to a probabilistic setting with more than one random variable.

A basis for the GNS-representation

Let us first construct the interacting Fock space representation $\mathcal{H}$ for a pair of free random variables a and b and some state φ. In general, this space should be generated by all non-commuting polynomials in a and b. In the previous section we showed how any univariate polynomial in either a or b can be decomposed as a linear combination of orthogonal polynomials in respectively a or b. So the Fock space $\mathcal{H}$ can likewise be shown to be the closure of

$$\mathrm{Span}\Big\{ p_{i_1}(a) q_{j_1}(b) \cdots p_{i_n}(a) q_{j_n} |\Omega\rangle \,|\, p_i, q_j \text{ orth. polynomials of } a \text{ and } b \Big\}. \tag{A.32}$$

Freeness of a and b also provides us with a basis for $\mathcal{H}$. The vectors

$$|i_1, j_1, \ldots, i_n, j_n\rangle \equiv p_{i_1}(a)q_{i_1}(b)\cdots p_{i_n}(a)q_{i_n}(b)\,|\Omega\rangle, \tag{A.33}$$

where the i_k and j_k are natural numbers and only i_1 and j_n can be zero, form an orthonormal set and from the above characterization of the interacting Fock space it should be clear that they are a generating set for $\mathcal{H}$.

Let us put this in a lemma,

Lemma A.1. *The set of vectors*

$$|i_1, i_2, \ldots, i_n\rangle, \qquad n \in \mathbb{N}, i_j \in \mathbb{Z}_0, \text{ and } \frac{i_j}{i_{j+1}} < 0 \tag{A.34}$$

defined by

$$|i_1, i_2, \ldots, i_n\rangle \equiv p^{\#}_{i_1}(\#)\cdots p^{\#}_{i_n}(\#)|\Omega\rangle, \tag{A.35}$$

where the $p^{\#}_{i_j}(\#)$ is the $i_j - th$ orthogonal polynomial associated to a if $i_j > 0$ and the $i_j - th$ orthogonal polynomial associated to b if $i_j < 0$, is a countable set and form a basis for the GNS-representation of a and b.

and prove it,

Proof. 1. *Normalization:* The conditions posed in (A.34) guarantee that the vectors $|i_1, \ldots, i_n\rangle$ are created by alternatingly applying an orthogonal polynomial in a and in b to the vacuum vector Ω. If we denote the orthogonal polynomials associated to a as p^+_i and the orthogonal polynomials associated to b as p^-_i, then

$$\||i_1, \ldots, i_n\rangle\| = |\langle i_n, \ldots, i_1 \,|\, i_1, \ldots, i_n\rangle|^2 \tag{A.36}$$

$$= |\langle\Omega|p^{sgn(i_n)}_{i_n}\cdots p^{sgn(i_2)}_{i_2}\left(p^{sgn(i_1)}_{i_1}\right)^2 p^{sgn(i_2)}_{i_2}\cdots p^{sgn(i_n)}_{i_n}|\Omega\rangle|^2. \tag{A.37}$$

This is the expectation value of an alternating sequence of polynomials in a and b which all have zero expectation under the vacuum state, except for the squared polynomial in the middle. If we replace

$$\left(p^{sgn(i_1)}_{i_1}\right)^2 \tag{A.38}$$

by

$$\left(p^{sgn(i_1)}_{i_1}\right)^2 - \langle\Omega|\left(p^{sgn(i_1)}_{i_1}\right)^2|\Omega\rangle, \tag{A.39}$$

the expectation of the resulting expression is zero since it is now an alternating sequence of polynomials in a and b with zero expectation. We can use this to rewrite (A.37) as

$$|\langle\Omega|p^{sgn(i_n)}_{i_n}\cdots p^{sgn(i_3)}_{i_3}\left(p^{sgn(i_2)}_{i_2}\right)^2 p^{sgn(i_3)}_{i_3}\cdots p^{sgn(i_n)}_{i_n}|\Omega\rangle|^2 \,.\, |\langle\Omega|\left(p^{sgn(i_1)}_{i_1}\right)^2|\Omega\rangle|^2. \tag{A.40}$$

Since we have normalized the polynomials $p^{\#}$, this reduces to

$$|\langle\Omega|p_{i_n}^{sgn(i_n)}\cdots p_{i_3}^{sgn(i_3)}\left(p_{i_2}^{sgn(i_2)}\right)^2 p_{i_3}^{sgn(i_3)}\cdots p_{i_n}^{sgn(i_n)}|\Omega\rangle|^2 \tag{A.41}$$

By iterating this calculation, we eventually find that the vectors $|i_1,\ldots,i_n\rangle$ are indeed normalized.

2. *Orthogonality:* A similar calculation allows us to rewrite

$$\langle i_1,\ldots,i_n\,|\,j_m,\ldots,j_1\rangle \tag{A.42}$$

as

$$\langle i_1,\ldots,i_{n-1}\,|\,j_{m-1},\ldots,j_1\rangle\cdot\langle i_n\,|\,j_m\rangle \tag{A.43}$$

If $i_n\neq j_m$, then the above expression is zero. If $i_n=j_m$, $\langle i_n\,|\,j_m\rangle=1$ and we reduce the problem by one order to the question whether

$$\langle i_1,\ldots,i_{n-1}\,|\,j_{m-1},\ldots,j_1\rangle =^{?} 0. \tag{A.44}$$

By iterating this process, we can conclude that

$$\langle i_1,\ldots,i_n\,|\,j_m,\ldots,j_1\rangle = 0 \tag{A.45}$$

iff the sequence $\mathbf{i}=(i_1,\ldots,i_n)$ is different from $\mathbf{j}=(j_1,\ldots,j_m)$.

3. *enumeration:*

   - If both a and b have a discrete spectrum, so that they have a finite number of orthogonal polynomials, say a has n orthogonal polynomials and b has m orthogonal polynomials, then we can interpret the sequence $\mathbf{i}$ as a natural number counted in base $(n+m)$. Since the length of any sequence $\mathbf{i}$ is finite, this representation of the natural numbers is unique. Ergo, this relation is a bijection and the set of vectors $|\mathbf{i}\rangle$ is is countable.
   - If the spectrum of a or b is not discrete, we can identify a sequence $\mathbf{i}$ with the rational number by concatenating the first $n-2$ numbers to obtain a signed natural number and interpreting the remaining pair as a rational number and adding this to the first number as the decimal part. This identification is unique, since both the concatenation and the map from pairs of natural number to the rational numbers can be made to be bijections. So, again we obtain that the set of vector $|\mathbf{i}\rangle$ is countable.

4. *completeness* follows from the observation at the start of this section that any polynomial in a and b can be rewritten in terms of sums and products of the orthogonal polynomials of a and b alone.

□

Jacobi matrix representation of random variables

As in section A.1 we can determine matrix-like descriptions for a and b in the GNS representation. Since we have defined a basis in our Hilbert space, we can now write a and b as

$$a = \sum_{\mathbf{i},\mathbf{j}} \langle \mathbf{i}|a|\mathbf{j}\rangle |\mathbf{i}\rangle\langle \mathbf{j}|, \tag{A.46}$$

$$b = \sum_{\mathbf{i},\mathbf{j}} \langle \mathbf{i}|b|\mathbf{j}\rangle |\mathbf{i}\rangle\langle \mathbf{j}|. \tag{A.47}$$

To determine the coefficients $\langle \mathbf{i}|a|\mathbf{j}\rangle$, we need to distinguish between the different cases which can arise. If

$$\langle \mathbf{i}|a|\mathbf{j}\rangle = \langle i_1,\ldots,i_n|a|j_m,\ldots,j_1\rangle, \tag{A.48}$$

then we can distinguish four different cases based on the signs of i_n and j_m:

- $\mathrm{sign}(i_n) > 0$ and $\mathrm{sign}(j_m) > 0$:

$$\begin{aligned} &\langle i_1,\ldots,i_n|a|j_m,\ldots,j_1\rangle && \text{(A.49)}\\ =&\langle i_1,\ldots,i_{n-1}\,|\,j_{m-1},\ldots,j_1\rangle \cdot \langle\Omega|p_{i_n}(a)ap_{j_m}(a)|\Omega\rangle && \text{(A.50)}\\ =&\delta_{\mathbf{i}(n-1),\mathbf{j}(m-1)}\big(\delta_{i_n,j_m+1}\alpha_{j_m} + \delta_{i_n,j_m}\beta_{(i_n+1)} + \delta_{i_n,j_m-1}\alpha_{i_n}\big) && \text{(A.51)} \end{aligned}$$

- $\mathrm{sign}(i_n) < 0$ and $\mathrm{sign}(j_m) > 0$:

$$\begin{aligned} &\langle i_1,\ldots,i_n|a|j_m,\ldots,j_1\rangle && \text{(A.52)}\\ =&\langle i_1,\ldots,i_n\,|\,j_{m-1},\ldots,j_1\rangle \cdot \langle\Omega|ap_{j_m}(a)|\Omega\rangle && \text{(A.53)}\\ =&\delta_{\mathbf{i},\mathbf{j}(m-1)}\big(\alpha_1\delta_{1,j_m}\big) && \text{(A.54)} \end{aligned}$$

- $\mathrm{sign}(i_n) < 0$ and $\mathrm{sign}(j_m) < 0$:

$$\langle i_1,\ldots,i_n|a|j_m,\ldots,j_1\rangle = \delta_{\mathbf{i},\mathbf{j}}\beta_1 \tag{A.55}$$

- $\mathrm{sign}(i_n) > 0$ and $\mathrm{sign}(j_m) < 0$:

$$\begin{aligned} &\langle i_1,\ldots,i_n|a|j_m,\ldots,j_1\rangle && \text{(A.56)}\\ =&\langle i_1,\ldots,i_{n-1}\,|\,j_m,\ldots,j_1\rangle \cdot \langle\Omega|p_{i_n}(a)a|\Omega\rangle && \text{(A.57)}\\ =&\delta_{\mathbf{i}(n-1),\mathbf{j}}\big(\alpha_1\delta_{1,i_n}\big) && \text{(A.58)} \end{aligned}$$

If a and b are both restricted to 4 distinct eigenvalues, we can represent them

on $\mathcal{H}$ as

$$a = \begin{pmatrix} \beta_1 & \alpha_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\ \alpha_1 & \beta_2 & \alpha_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\ 0 & \alpha_2 & \beta_3 & \alpha_3 & 0 & 0 & 0 & 0 & 0 & 0 & \\ 0 & 0 & \alpha_3 & \beta_4 & 0 & 0 & 0 & 0 & 0 & 0 & \\ 0 & 0 & 0 & 0 & \beta_1 & 0 & 0 & \alpha_1 & 0 & 0 & \\ 0 & 0 & 0 & 0 & 0 & \beta_1 & 0 & 0 & 0 & 0 & \\ 0 & 0 & 0 & 0 & 0 & 0 & \beta_1 & 0 & 0 & 0 & \\ 0 & 0 & 0 & 0 & \alpha_1 & 0 & 0 & \beta_2 & \alpha_2 & 0 & \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha_2 & \beta_3 & \alpha_3 & \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha_3 & \beta_4 & \\ & & & & & & & & & & \ddots \end{pmatrix}, \tag{A.59}$$

$$b = \begin{pmatrix} \gamma_1 & 0 & 0 & 0 & \kappa_1 & 0 & 0 & 0 & 0 & 0 & \\ 0 & \gamma_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\ 0 & 0 & \gamma_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\ 0 & 0 & 0 & \gamma_1 & 0 & 0 & 0 & 0 & 0 & 0 & \\ \kappa_1 & 0 & 0 & 0 & \gamma_2 & \kappa_2 & 0 & 0 & 0 & 0 & \\ 0 & 0 & 0 & 0 & \kappa_2 & \gamma_3 & \kappa_3 & 0 & 0 & 0 & \\ 0 & 0 & 0 & 0 & 0 & \kappa_3 & \gamma_4 & 0 & 0 & 0 & \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \gamma_1 & 0 & 0 & \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \gamma_1 & 0 & \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \gamma_1 & \\ & & & & & & & & & & \ddots \end{pmatrix} \tag{A.60}$$

These matrices are just reshuffled versions of infinite repetitions of the matrix representation we constructed in

In the same way, we can also reshuffle the sum of a and b to a more useful form

$$a + b = \begin{pmatrix} \beta_1 + \gamma_1 & \alpha_1 & \kappa_1 & & & & \\ \alpha_1 & \beta_2 + \gamma_1 & 0 & \alpha_2 & \kappa_2 & & \\ \kappa_1 & 0 & \beta_1 + \gamma_2 & 0 & 0 & \alpha_3 & \kappa_3 \\ & \alpha_2 & 0 & \beta_3 + \gamma_1 & 0 & & \end{pmatrix} \tag{A.61}$$

Representation of free random variables on interacting Fock spaces

Since we have proven that the GNS-representation space $\mathcal{H}$ is an infinite-dimensional separable Hilbert space, we can on general grounds state that an isomorphism between this space $\mathcal{H}$ and some interacting Fock space exists. Such an isomorphism is elucidated in the following lemma.

Lemma A.2. *The Hilbert space $\mathcal{H}$ associated to the GNS-representation of two free random variables is isomorphic to an interacting Fock space $\mathcal{F}(\mathcal{K})$ where $\mathcal{K}$ is a two-dimensional Hilbert space.*

Proof. Let us first recall the explicit construction of an (interacting) Fock space based on a one-particle Hilbert space $\mathcal{K}$. The Fock space is then,

$$\mathcal{F}(\mathcal{K}) = \oplus_0^\infty \mathcal{K}^n, \tag{A.62}$$

where

$$\mathcal{K}^n = \otimes^n K \qquad \forall n > 0, \tag{A.63}$$

$$\mathcal{K}^0 = \mathbb{C}. \tag{A.64}$$

If the Hilbert space $\mathcal{K}$ is spanned by the vectors k_1 and k_2, the set

$$\{k_{i_1} \otimes \cdots \otimes k_{i_n} \,|\, i_j = 1, 2 \,\forall j \leq n, n \in \mathbb{N}\} \tag{A.65}$$

is a basis for $\mathcal{F}(\mathcal{K})$.

The map $U : \mathcal{H} \to \mathcal{F}(\mathcal{K})$

$$U : |\mathbf{i} = (i_1, \ldots, i_n)\rangle \mapsto \underbrace{k_{\#_{i_1}} \otimes \cdots \otimes k_{\#_{i_1}}}_{i_1 times} \otimes \cdots \otimes \underbrace{k_{\#_{i_n}} \otimes \cdots \otimes k_{\#_{i_n}}}_{i_n times}, \tag{A.66}$$

where $\#_j = 1$ if $j > 0$ and $\#_j = 2$ if $j < 0$, is a bijection between the basis of $\mathcal{H}$ and $\mathcal{F}(\mathcal{K})$ and thus extends to an isomorphism between $\mathcal{H}$ and $\mathcal{F}(\mathcal{K})$.

□

In section A.2 we have described the operators a and b in terms of the basis vectors $|\mathbf{i}\rangle$. We can now use the above isomorphism arising from the map U to transport the operators a and b to the interacting Fock space.

Lemma A.3. *The map $\pi : \mathcal{A} \to \mathcal{F}(\mathcal{K})$ defined by*

$$\pi : a \mapsto S_a + D_a + S_a^*, \tag{A.67}$$

$$\pi : b \mapsto S_b + D_b + S_b^*, \tag{A.68}$$

where

$$S_a |k_{i_1} \otimes k_{i_n}\rangle = \alpha \tag{A.69}$$

is an homomorphism.

APPENDIX B

Various proofs

B.1 proof of lemma 4.5

Lemma B.1. *Let V be a Hermitian operator in some C^*-algebra. Inside a sphere with radius $(6\|V\|)^{-1}$, the free cumulant series $K_V(w)$ converges to a bounded, analytic function. Moreover, K_V maps $\mathcal{D}^+ := \mathcal{D} \cap \mathbb{C}^+$ to $\mathcal{D}^+$ and $\mathcal{D}^- := \mathcal{D} \cap \mathbb{C}^-$ to $\mathcal{D}^-$.*

-

Proof. We first introduce a better estimate for the domain $\mathcal{D}$ where the cumulant series K_V is analytic. In [66], it was established that K_V extends uniquely to an analytic function on the domain $\mathcal{D} = \{w \,|\, w \leq (6\|V\|)^{-1}\}$.

In remark 4.4, we established a relation between the formal inverse $G_V^{\langle -1 \rangle}$ and the cumulant series of V,

$$K_V(w) = G_V^{\langle -1 \rangle}(w) - \frac{1}{w}. \tag{B.1}$$

On the same domain $\mathcal{D}$ that K_V is analytic, $G^{\langle -1 \rangle}$ is meromorphic with a single simple pole at $w = 0$. On the domain $\mathcal{D}$, the relation between K_V and $G_V^{\langle -1 \rangle}$ thus also holds on the level of complex functions. This allows us to study more closely how K_V behaves on the domain $\mathcal{D}$.

In [68] we found the following proposition,

Proposition B.2. *Let F be holomorphic on $\mathbb{C}^+ \to \mathbb{C}^+$. A necessary and sufficient condition for F to be the multiplicative inverse of a Cauchy transform of some*

probability measure μ on $\mathbb{R}$ is that

$$\inf_{z\in\mathbb{C}^+} \frac{Im\, F(z)}{Im\, z} = 1. \tag{B.2}$$

In particular, every such F increases the imaginary part:

$$Im\, F(z) \geq Im\, z. \tag{B.3}$$

In the notation of this chapter, this means that

$$\operatorname{Im} \frac{1}{G_V(z)} \geq \operatorname{Im} z, \quad \forall\, z \in \mathbb{C}^+, \quad \operatorname{Im} \frac{1}{G_V(z)} \leq \operatorname{Im} z, \quad \forall\, z \in \mathbb{C}^-. \tag{B.4}$$

In particular, if z is such that $G_V(z) \in \mathcal{D}$, then there exists a unique w such that $G^{\langle -1\rangle}(w) = z$. The above behavior of G_V then translates to,

$$\operatorname{Im} \frac{1}{w} \geq \operatorname{Im} G_V^{\langle -1\rangle}(w) \geq 0, \quad \forall\, w \in \mathcal{D}^- := \mathcal{D} \cap \mathbb{C}^-, \tag{B.5}$$

$$\operatorname{Im} \frac{1}{w} \leq \operatorname{Im} G_V^{\langle -1\rangle}(w) \leq 0, \quad \forall\, w \in \mathcal{D}^+ := \mathcal{D} \cap \mathbb{C}^+. \tag{B.6}$$

Since $\operatorname{Im} K_V(w) = \operatorname{Im} G_V^{\langle -1\rangle}(w) - \operatorname{Im} \frac{1}{w}$, the above means that K_V maps $\mathcal{D}^+$ onto $\mathcal{D}^+$ and $\mathcal{D}^-$ to $\mathcal{D}^-$.

□

B.2 Proof of lemma 4.13

Lemma B.3. *Let H be the Hamiltonian of a dynamical model as proposed in section 4.1.2, so that H can be written as $H_0 + V$, where V is free from H_0 in the probability space $(\mathcal{S} \otimes \mathcal{E}, \tau)$. In a neighborhood of ∞, the two point function $\mathbf{r}(z_1, z_2)$,*

$$\mathbf{r}(z_1, z_2) = \mathbb{E}\left[\frac{1}{z_1 - H} \left(\sigma(0) \otimes \mathsf{E}\right) \frac{1}{z_2 - H} \right], \tag{B.7}$$

is amenable to a description in terms of the rescaled conditionally expected resolvent mapping of H,

$$\mathbf{r}(z_1, z_2) = \frac{\mathbf{r}(z_1) - \mathbf{r}(z_2)}{z_2 - z_1} \times \frac{K_V\left(r(z_1)\right) - K_V\left(r(z_2)\right)}{r(z_1) - r(z_2)} \tag{B.8}$$

$$\times \operatorname{Tr} \mathbb{E}\left[\frac{1}{z_1 - K_V(r(z_1)) - H_0} (\sigma(0) \otimes \mathsf{E}) \frac{1}{z_2 - K_V(r(z_2)) - H_0} \right] \tag{B.9}$$

$$+ \mathbb{E}\left[\frac{1}{z_1 - K_V(r(z_1)) - H_0} (\sigma(0) \otimes \mathsf{E}) \frac{1}{z_2 - K_V(r(z_2)) - H_0} \right]. \tag{B.10}$$

-

Proof. A similar technique as was used in section 4.3 to calculate the reduced resolvent mapping of H can then be used to calculate explicitly the two-point function $\mathbf{r}(z_1, z_2)$,

$$\mathbf{r}(z_1, z_2) := \mathbb{E}\left[\frac{1}{z_1 - H}\,(\sigma(0) \otimes \mathsf{E})\,\frac{1}{z_2 - H}\right]. \tag{B.11}$$

As in the case of the Hamiltonian specter, it is convenient to introduce a specific notation for the trace of $\mathbf{r}(z_1, z_2)$

$$r(z_1, z_2) = \operatorname{Tr}\mathbb{E}\left[\frac{1}{z_1 - H}\,(\sigma(0) \otimes \mathsf{E})\,\frac{1}{z_2 - H}\right]. \tag{B.12}$$

To make the two-point function more amenable to our probabilistic framework, we need to translate it to the probability space $(\mathcal{S} \otimes \mathcal{E}, \tau)$,

$$\mathbf{r}_{ij}(z_1, z_2) = \tau\left[(E_{ji} \otimes \mathbb{1}_{\mathcal{E}})\frac{1}{z_1 - H}\,(\mathsf{S} \otimes \mathsf{E})\,\frac{1}{z_2 - H}\right]. \tag{B.13}$$

As was indicated in section 4.3, the rescaled expectation $r(z)$ is the essential ingredient in this reduced description. The following lemma describes how the two-point function $\mathbf{r}(z_1, z_2)$ can be written as a function of the (one-point) function $r(z)$.

This can be reformulated in terms of the non-interacting Hamiltonian H_0 and the interaction term V,

$$\mathbf{r}_{ij}(z_1, z_2) = \tau\left[(E_{ji} \otimes \mathbb{1}_{\mathcal{E}})\frac{1}{z_1 - H_0 - V}\,(\mathsf{S} \otimes \mathsf{E})\,\frac{1}{z_2 - H_0 - V}\right]. \tag{B.14}$$

For sufficiently large $|z_1|$ and $|z_2|$, we can expand the resolvents in this expression as Neumann series,

$$\mathbf{r}_{ij}(z_1, z_2) = \sum_{n_1, n_2 = 0}^{\infty} \tau\Big[(E_{ji} \otimes \mathbb{1}_{\mathcal{E}})(z_1 - H)^{-1}\left(V(z_1 - H_0)^{-1}\right)^{n_1} \tag{B.15}$$

$$\times\,(\mathsf{S} \otimes \mathsf{E})\,(z_2 - H)^{-1}\left(V(z_2 - H_0)^{-1}\right)^{n_2}\Big] \tag{B.16}$$

To conserve some real estate, we write $A_i = (z_i - H_0)^{-1}$, $A_k^{(ij)} = (E_{ji \otimes \mathbb{1}_{\mathcal{E}}})(z_k - H_0)^{-1}$ and $\mathsf{S} \otimes \mathsf{E} = M$,

$$\mathbf{r}_{ij}(z_1, z_2) = \sum_{n_1, n_2 = 0}^{\infty} \tau\left[A_1^{(ij)}\,(VA_1)^{n_1}\,MA_2\,(VA_2)^{n_2}\right]. \tag{B.17}$$

This looks similar to the expressions encountered in the proof of theorem 4.2, so it seems plausible that an adaptation of the proof there might work here as well.

For this scheme to work, we need to rewrite this expressions somewhat so that we always have at least one V at our disposal in the summation,

$$\mathbf{r}_{ij}(z_1, z_2) = \tau\left[A_1^{(ij)} M A_2 (VA)^{n_2}\right] + \sum_{\substack{n_1=1,\\ n_2=0}}^{\infty} \tau\left[A_1^{(ij)} (VA_1)^{n_1} M A_2 (VA_2)^{n_2}\right]. \tag{B.18}$$

The first term can recombined into a fractional form,

$$\tau\left[A_1^{(ij)} M A_2 (VA_2)^{n_2}\right] = \tau\left[A_1^{(ij)} M \frac{1}{A_2^{-1} - V}\right]. \tag{B.19}$$

For the moment, we put this term to the side and concentrate on the remaining summation,

$$\sum_{\substack{n_1=1,\\ n_2=0}}^{\infty} \tau\left[A_1^{(ij)} (VA_1)^{n_1} M A_2 (VA_2)^{n_2}\right], \tag{B.20}$$

or since τ is tracial,

$$\sum_{\substack{n_1=1,\\ n_2=0}}^{\infty} \tau\left[(VA_1)^{n_1} M A_2 (VA_2)^{n_2} A_1^{(ij)}\right], \tag{B.21}$$

This can be rewritten in terms of free cumulants as,

$$\sum_{\substack{n_1=1,\\ n_2=0}}^{\infty} \sum_{\pi \in NC(2(n_1+n_2)+3)} \tag{B.22}$$

$$k_\pi\left(\dot{V}, A_1, \underbrace{V, A_1, \ldots, V, A_1}_{(n_1-1 \text{ times})}, M, A_2, \underbrace{V, A_2, \ldots, V, A_2}_{(n_2 \text{ times})}, A_1^{(ij)}\right) \tag{B.23}$$

We can rearrange the terms in the sum over $NC(2(n_1 + n_2) + 3)$ according to the number of elements connected by the bridge that starts at the dotted V, the first V which appears in the above expansion. Since A_k and V, as well as M and V are free, the only non-zero cumulants are those which correspond to partitions where the bridges connect only $A's$ and M or only V's. For any n_1, n_2 there are exactly $(n_1 + n_2)$ V's, so the bridge that contains $\dot{V}$ connects at most $(n_1 + n_2)$ elements.

Compared to the proof of theorem 4.2, there is now an added complication. $\dot{V}$ can be connected only to V's occurring before M in the above expression or it can jump the fence and also connect to V's after M. These two situations correspond to qualitatively different expressions, so we prepare for this by splitting the summation

over W_1 as it was used in the proof of theorem 4.2 into a summation over two subsets of W_1, X and Y. The subset X collects all indices which correspond to the V's connected to $\dot{V}$ which occur before M and Y collects all the indices which correspond to V's connected to $\dot{V}$ which occur after M. By construction, the set X contains at least one element, the index 1. It contains at most n_1 elements and is a subset of the circle segment $[1\,,\,2n_1-1]$. The set Y can be empty, contains at most n_2 elements and is a subset of the circle segment $[2n_1+3\,,\,2(n_1+n_2)+1]$. We can inject this structure into (B.22),

$$\sum_{\substack{n_1=1,\\ n_2=0}}^{\infty}\sum_{s=1}^{n_1}\sum_{t=0}^{n_2}\sum_{\substack{X,\\ |X|=s,\,1\in X,\\ X\subset[1,2n_1-1].}}\sum_{\substack{Y,\,|Y|=t,\\ Y\subset[2n_1+3,2(n_1+n_2)+1].}}\sum_{\substack{\pi\in NC(2n_1+2n_2+3)\\ \pi=\{X\cup Y,\ldots\}}} \tag{B.24}$$

$$k_\pi\left(\dot{V},A_1,\underbrace{V,A_1,\ldots,V,A_1}_{(n_1-1\text{ times})},M,A_2,\underbrace{V,A_2,\ldots,V,A_2}_{(n_2\text{ times})},A_1^{(ij)}\right) \tag{B.25}$$

If $X=\{x_1,\ldots,x_s\}$, $Y=\{y_1,\ldots,y_t\}$ and $y_{t+1}:=2(n_1+n_2)+4$, then π can be further decomposed as

$$\pi=(X\hat{\cup}Y)\cup\sigma_1\cup\cdots\sigma_{(s-1)}\cup\mu\cup\gamma_1\cup\cdots\gamma_t, \tag{B.26}$$

such that σ_k $(k<s)$ is a non-crossing partition of $\{x_k+1,x_k+2,\ldots,x_{k+1}-1\}$, μ is a non-crossing partition of $\{x_s+1,x_s+2,\ldots,y_1-1\}$ and γ_k $(k\leq t)$ is a non-crossing partition of $\{y_k+1,y_k+2,\ldots,y_{k+1}-1\}$. We gave the $\cup$ in $X\hat{\cup}Y$ a hat, to signify[1] that its meaning is different from the other $\cup$ signs. $X\hat{\cup}Y$ is a union of index-sets, which indicate to which V's, $\dot{V}$ is connected. The other $\cup$ signs indicate the disjoint union of partitions of subsets to form a partition of the disjoint union of the subsets.

We make a distinction between the partitions σ_k, γ_k and μ based on their arguments. Any σ_k has as arguments a series of the form,

$$A_1,V,A_1,\ldots,V,A_1, \tag{B.27}$$

any γ_k $(k<t)$ has as arguments a series of the form,

$$A_2,V,A_2,\ldots,V,A_2, \tag{B.28}$$

γ_t has an argument of the form

$$A_2,V,A_2,\ldots,V,A_2,A_1^{(ij)}, \tag{B.29}$$

and μ has as arguments a series of the form,

$$A_1,V,A_1,\ldots,V,A_1,M,A_2,V,A_2,\ldots,V,A_2, \tag{B.30}$$

[1] Also, hats seem to be all the rage this winter.

or

$$A_1, V, A_1, \ldots, V, A_1, M, A_2, V, A_2, \ldots, V, A_2, A_1^{(ij)}, \tag{B.31}$$

if $t = 0$. With this information, equation (B.24) can be rewritten as

$$\sum_{\substack{n_1=1,\\ n_2=0}}^{\infty} \sum_{s=1}^{n_1} \sum_{t=0}^{n_2} \sum_{\substack{X,\\ |X|=s, 1\in X,\\ X\subset[1,2n_1-1]}} \sum_{\substack{Y,\\ |Y|=t,\\ Y\subset[2n_1+3,2(n_1+n_2)+1]}} \sum_{\substack{\pi\in NC(2n_1+2n_2+3)\\ \pi=\{X\hat{\cup}Y,\ldots\}}} \tag{B.32}$$

$$k_{s+t}(\dot{V},\ldots,V) k_{\sigma_1}(A_1, \underbrace{V, A_1, \ldots, V, A_1}_{(x_2-x_1-2)/2 \text{ times}}) \cdots k_{\sigma_{s-1}}(A_1, \underbrace{V, A_1, \ldots, V, A_1}_{(x_s-x_{s-1}-2)/2 \text{ times}}) \tag{B.33}$$

$$\times k_\mu(A_1, \underbrace{V, A_1, \ldots, V, A_1}_{(2n_1-x_s-1)/2 \text{ times}}, M, A_2, \underbrace{V, A_2, \ldots, V, A_2}_{(y_1-2n_1-3)/2 \text{ times}}, (A_1^{(ij)})^{(1-\delta_{0,t})}) \tag{B.34}$$

$$\times k_{\gamma_1}(A_2, \underbrace{V, A_2, \ldots, V, A_2}_{(y_2-y_1-2)/2 \text{ times}}) \cdots k_{\gamma_t}(A_2, \underbrace{V, A_2, \ldots, V, A_2}_{(y_{t+1}-y_t-2)/2 \text{ times}}, A_1^{(ij)}). \tag{B.35}$$

This rather large sum can be rewritten in terms of the elements of X and Y and appropriate conditions on the σ's, μ and the γ's,

$$\sum_{\substack{n_1=1,\\ n_2=0}}^{\infty} \sum_{s=1}^{n_1} \sum_{t=0}^{n_2} \sum_{\substack{(1,x_2,\ldots,x_s),\\ x_s\le 2n_1-1}} \sum_{\substack{(y_1,\ldots,y_t),\\ 2n_1+3\le y_1,\, y_t\le 2(n_1+n_2)+1}} \tag{B.36}$$

$$\sum_{\sigma_k\in NC([x_k+1,x_{k+1}-1])} \sum_{\mu\in NC([x_s+1,y_1-1])} \sum_{\gamma_k\in NC([y_k+1,y_{k+1}-1])} k_{\ldots}. \tag{B.37}$$

All terms and factors in this expression depend only on the difference of sequential x_k's and y_k's, and not their absolute values. If we put

$$i_k := \begin{cases} (x_{k+1}-x_k-2)/2 & \text{if} \quad 1\le k<s, \\ (2n_1-x_k-1)/2 & \text{if} \quad k=s, \\ (y_1-2n_1-3)/2 & \text{if} \quad k=s+1, \\ (y_{k-s}-y_{k-s-1}-2)/2 & \text{if} \quad s+2\le k\le s+t+1, \end{cases} \tag{B.38}$$

(B.36) becomes,

$$\sum_{\substack{n_1=1,\\ n_2=0}}^{\infty}\sum_{s=1}^{n_1}\sum_{t=0}^{n_2}\sum_{\substack{i_1,\ldots,i_s\in\\ \{0,\ldots,n_1-1\}\\ i_1+\cdots+i_s=n_1-s}}\sum_{\substack{i_{s+1},\ldots,i_{s+t+1}\in\\ \{0,\ldots,n_2-1\}\\ i_{s+1}+\cdots+i_{s+t+1}=n_2-t}}\sum_{\substack{\nu_k\in\\ NC(2i_k+1)}} \tag{B.39}$$

$$k_{s+t}(\dot{V},\ldots,V)k_{\nu_1}(A_1,\underbrace{V,A_1,\ldots,V,A_1}_{i_1\text{ times}})\cdots k_{\nu_{s-1}}(A_1,\underbrace{V,A_1,\ldots,V,A_1}_{i_{s-1}\text{ times}}) \tag{B.40}$$

$$\times k_{\nu_s}\Big(A_1,\underbrace{V,A_1,\ldots,V,A_1}_{i_s\text{ times}},M,A_2,\underbrace{V,A_2,\ldots,V,A_2}_{i_{(s+1)}\text{ times}},(A_1^{(ij)})^{(1-\delta_{0,t})}\Big) \tag{B.41}$$

$$\times k_{\nu_{s+1}}(A_2,\underbrace{V,A_2,\ldots,V,A_2}_{i_{(s+2)}\text{ times}})\cdots k_{\nu_{s+t}}(A_2,\underbrace{V,A_2,\ldots,V,A_2}_{i_{(s+t+1)}\text{ times}},A_1^{(ij)}). \tag{B.42}$$

The factors in this last expression still have a rather complicated dependence on t. This can be mediated somewhat by splitting up the summation over t as

$$\sum_{t=0}^{n_2}\text{terms}(t)=\text{term}(t=0)+\text{term}(t=1)+\sum_{t=2}^{n_2}\text{terms}(t), \tag{B.43}$$

when n_2 is large enough to sustain such a decomposition. The term for $t=0$ appears for all values of n_2, so in light of the proof of theorem 4.2,

$$\sum_{n_1=1,n_2=0}^{\infty}\sum_{s=1}^{n_1}\sum_{\substack{i_1,\ldots,i_s\in\\ \{0,\ldots,n_1-1\}\\ i_1+\cdots+i_s=n_1-s}}\sum_{\substack{\nu_k\in\\ NC(2i_k+1)}} \tag{B.44}$$

$$k_s(\dot{V},\ldots,V)k_{\nu_1}(A_1,\underbrace{V,A_1,\ldots,V,A_1}_{i_1\text{ times}})\cdots k_{\nu_{s-1}}(A_1,\underbrace{V,A_1,\ldots,V,A_1}_{i_{s-1}\text{ times}}) \tag{B.45}$$

$$\times k_{\nu_s}\Big(A_1,\underbrace{V,A_1,\ldots,V,A_1}_{i_s\text{ times}},M,A_2,\underbrace{V,A_2,\ldots,V,A_2}_{n_2\text{ times}},A_1^{(ij)}\Big) \tag{B.46}$$

$$\tag{B.47}$$

$$=\sum_{s=1}^{\infty}k_s(\dot{V},\ldots,V)r(z_1)^{s-1}\times\tau\left[A_1^{(ij)}\frac{1}{A_1^{-1}-V}\,M\,\frac{1}{A_2^{-1}-V}\right] \tag{B.48}$$

$$=K_V\left(r(z_1)\right)\times\tau\left[A_1^{(ij)}\frac{1}{A_1^{-1}-V}\,M\,\frac{1}{A_2^{-1}-V}\right] \tag{B.49}$$

$$:=K\times\tau\left[A_1^{(ij)}\frac{1}{A_1^{-1}-V}\,M\,\frac{1}{A_2^{-1}-V}\right] \tag{B.50}$$

The $(t=1)$-term appears for all $n_2 \geq 1$,

$$\sum_{\substack{n_1=1,\\ n_2=1}}^{\infty} \sum_{s=1}^{n_1} \sum_{\substack{i_1,\ldots,i_s\in\\ \{0,\ldots,n_1-1\}\\ i_1+\cdots+i_s=n_1-s}} \sum_{\substack{i_{s+1}\in\\ \{0,\ldots,n_2-1\}}} \sum_{\substack{\nu_k\in\\ NC(2i_k+1)}} \tag{B.51}$$

$$k_{(s+1)}(\dot{V},\ldots,V)k_{\nu_1}(A_1,\underbrace{V,A_1,\ldots,V,A_1}_{i_1 \text{ times}})\cdots k_{\nu_{s-1}}(A_1,\underbrace{V,A_1,\ldots,V,A_1}_{i_{(s-1)} \text{ times}}) \tag{B.52}$$

$$\times k_{\nu_s}(A_1,\underbrace{V,A_1,\ldots,V,A_1}_{i_s \text{ times}},M,A_2,\underbrace{V,A_2,\ldots,V,A_2}_{i_{(s+1)} \text{ times}}) \tag{B.53}$$

$$\times k_{\nu_{(s+1)}}(A_2,\underbrace{V,A_2,\ldots,V,A_2}_{n_2-i_{(s+1)}-1 \text{ times}},A_1^{(ij)}) \tag{B.54}$$

$$=\sum_{s=1}^{\infty} k_{(s+1)}(\dot{V},\ldots,V)r(z_1)^{s-1}\times r(z_1,z_2)\times\tau\left[A_1^{(ij)}\frac{1}{A_2^{-1}-V}\right]. \tag{B.55}$$

The rest of the terms in the summation over t can collected as,

$$\sum_{\substack{n_1=1,\\ n_2=2}}^{\infty} \sum_{s=1}^{n_1}\sum_{t=2}^{n_2} \sum_{\substack{i_1,\ldots,i_s\in\\ \{0,\ldots,n_1-1\}\\ i_1+\cdots+i_s=n_1-s}} \sum_{\substack{i_{s+1},\ldots,i_{s+t+1}\in\\ \{0,\ldots,n_2-1\}\\ i_{s+1}+\cdots+i_{s+t+1}=n_2-t}} \sum_{\substack{\nu_k\in\\ NC(2i_k+1)}} \tag{B.56}$$

$$k_{s+t}(\dot{V},\ldots,V)k_{\nu_1}(A_1,\underbrace{V,A_1,\ldots,V,A_1}_{i_1 \text{ times}})\cdots k_{\nu_{s-1}}(A_1,\underbrace{V,A_1,\ldots,V,A_1}_{i_{s-1} \text{ times}}) \tag{B.57}$$

$$\times k_{\nu_s}\Big(A_1,\underbrace{V,A_1,\ldots,V,A_1}_{i_s \text{ times}},M,A_2,\underbrace{V,A_2,\ldots,V,A_2}_{i_{(s+1)} \text{ times}}\Big) \tag{B.58}$$

$$\times k_{\nu_{s+1}}(A_2,\underbrace{V,A_2,\ldots,V,A_2}_{i_{(s+2)} \text{ times}})\cdots k_{\nu_{s+t}}(A_2,\underbrace{V,A_2,\ldots,V,A_2}_{i_{(s+t+1)} \text{ times}},A_1^{(ij)}) \tag{B.59}$$

$$=\sum_{s=1}^{\infty}\sum_{t=2}^{\infty} k_{(s+t)}(\dot{V},\ldots,V)r(z_1)^{s-1}\,r(z_2)^{t-1}\times\tau\left[A_1^{(ij)}\frac{1}{A_2^{-1}-V}\right]\times r(z_1,z_2). \tag{B.60}$$

If we add the $(t=1)$ and $(t>1)$-terms together, this becomes

$$\sum_{s=1}^{\infty}\sum_{t=1}^{\infty} k_{(s+t)}(\dot{V},\ldots,V)r(z_1)^{s-1}\,r(z_2)^{t-1}\times\tau\left[A_1^{(ij)}\frac{1}{A_2^{-1}-V}\right]\times r(z_1,z_2), \tag{B.61}$$

$$:= L\times\tau\left[A_1^{(ij)}\frac{1}{A_2^{-1}-V}\right]. \tag{B.62}$$

The grand total of all these terms is,

$$\tau\left[A_1^{(ij)} M \frac{1}{A_2^{-1}-V}\right] + L\,\tau\left[A_1^{(ij)} \frac{1}{A_2^{-1}-V}\right] + K\,\tau\left[A_1^{(ij)} \frac{1}{A_1^{-1}-V} M \frac{1}{A_2^{-1}-V}\right]. \tag{B.63}$$

This expression can again be used as a starting point for an iteration procedure which results in

$$\sum_{n=0}^{\infty} K^n \times \tau\left[A_1^{(ij)} A_1^n M \frac{1}{A_2^{-1}-V}\right] + LK^n \times \tau\left[A_1^{(ij)} A_1^n \frac{1}{A_2^{-1}-V}\right]. \tag{B.64}$$

These summations are equivalent to Neumann series, so we can rewrite this as

$$\tau\left[(E_{ji}\otimes \mathbb{1}_E)\frac{1}{A_1^{-1}-K} M \frac{1}{A_2^{-1}-V}\right] + L \times \tau\left[(E_{ji}\otimes \mathbb{1}_E)\frac{1}{A_1^{-1}-K}\ \frac{1}{A_2^{-1}-V}\right].$$

If we now use theorem 4.2 one last time to get rid of the final V's appearing in this equation, we end up with a self-consistent equation for our reduced two-point function,

$$\begin{aligned} r_{ij}(z_1,z_2) &= \tau\left[(E_{ji}\otimes \mathbb{1}_{\mathcal{E}})\frac{1}{z_1 - K_V(r(z_1)) - H_0}\ \frac{1}{z_2 - K_V(r(z_2)) - H_0}\right] \\ &\times \sum_{s,t=1}^{\infty} k_{(s+t)}(\dot{V},\ldots,V) r(z_1)^{s-1}\, r(z_2)^{t-1} \times r(z_1,z_2) \\ &+ \tau\left[(E_{ji}\otimes \mathbb{1}_{\mathcal{E}})\frac{1}{z_1 - K_V(r(z_1)) - H_0}(\mathsf{S}\otimes \mathsf{E})\frac{1}{z_2 - K_V(r(z_2)) - H_0}\right]. \end{aligned}$$

The factor

$$\tilde{L} = \sum_{s,t=1}^{\infty} k_{(s+t)}(\dot{V},\ldots,V) r(z_1)^{s-1}\, r(z_2)^{t-1}$$

is either calculate directly through the general identity $a^n - b^n = (a-b)(\sum \cdots)$ or we can leverage the self-consistent equation for the reduced two-point function to rewrite $\tilde{L}$ in a more manageable form[2]. Notice that this factor is independent of the operator $\mathsf{S}\otimes\mathsf{E}$. For $\mathsf{S}\otimes\mathsf{E} = \mathbb{1}$, $r(z_1,z_2)$ can be calculated directly as

$$r(z_1,z_2) = \frac{1}{z_2 - z_1}\,\tau\left[\frac{1}{z_1 - H} - \frac{1}{z_2 - H}\right] = \frac{r(z_1) - r(z_2)}{z_2 - z_1}. \tag{B.65}$$

[2]In this way, we get some reassurance that we have not made any mistakes up to now.

The self-consistent equation we derived above should still be applicable, so $r(z_1, z_2)$ can also be expressed as

$$r(z_1, z_2) = \tau \left[\frac{1}{z_1 - K_V(r(z_1)) - H_0} \frac{1}{z_2 - K_V(r(z_2)) - H_0} \right] \tag{B.66}$$

$$+ \tau \left[\frac{1}{z_1 - K_V(r(z_1)) - H_0} \frac{1}{z_2 - K_V(r(z_2)) - H_0} \right] \tag{B.67}$$

$$\times \sum_{s,t=1}^{\infty} k_{(s+t)}(\dot{V}, \ldots, V) r(z_1)^{s-1} r(z_2)^{t-1} \times r(z_1, z_2) \tag{B.68}$$

which includes the complicated $\tilde{L}$-factor. The residual two-point functions $r(z_1, z_2)$ can be expanded out using the identity established in (B.65). Similarly, the expectation value

$$\tau \left[\frac{1}{z_1 - K_V(r(z_1)) - H_0} \frac{1}{z_2 - K_V(r(z_2)) - H_0} \right] \tag{B.69}$$

can be rewritten in terms of one-point functions as,

$$\frac{r(z_1) - r(z_2)}{z_2 - z_1 + K_V(r(z_1)) - K_V(r(z_2))}. \tag{B.70}$$

If we also substitute this identity in (B.66), we can rewrite $\tilde{L}$ as,

$$\tilde{L} = \sum_{s,t=1}^{\infty} k_{(s+t)}(\dot{V}, \ldots, V) r(z_1)^{s-1} r(z_2)^{t-1} = \frac{K_V\left(r(z_1)\right) - K_V\left(r(z_2)\right)}{r(z_1) - r(z_2)}. \tag{B.71}$$

which is of course the same as what we would have obtained by direct application of the factoring identity and rather reassuring.

If we input this identity for the factor $\tilde{L}$, the self-consistent equation for $\mathbf{r}_{ij}(z_1, z_2)$ simplifies to,

$$\mathbf{r}_{ij}(z_1, z_2) = \tau \left[(E_{ji} \otimes \mathbb{1}_{\mathcal{E}}) \frac{1}{z_1 - K_V(r(z_1)) - H_0} \frac{1}{z_2 - K_V(r(z_2)) - H_0} \right] \tag{B.72}$$

$$\times \frac{K_V\left(r(z_1)\right) - K_V\left(r(z_2)\right)}{r(z_1) - r(z_2)} \times r(z_1, z_2) \tag{B.73}$$

$$+ \tau \left[(E_{ji} \otimes \mathbb{1}_{\mathcal{E}}) \frac{1}{z_1 - K_V(r(z_1)) - H_0} (\mathsf{S} \otimes \mathsf{E}) \frac{1}{z_2 - K_V(r(z_2)) - H_0} \right]. \tag{B.74}$$

The factor $r(z_1, z_2)$ in this expression satisfies its own self-consistent equation which

can be recovered from the above equation by summing up all the terms $\mathbf{r}_{ii}(z_1, z_2)$,

$$r(z_1, z_2) = \tau \left[\frac{1}{z_1 - K_V(r(z_1)) - H_0} \frac{1}{z_2 - K_V(r(z_2)) - H_0} \right] \tag{B.75}$$

$$\times \frac{K_V\left(r(z_1)\right) - K_V\left(r(z_2)\right)}{r(z_1) - r(z_2)} \times r(z_1, z_2) \tag{B.76}$$

$$+ \tau \left[\frac{1}{z_1 - K_V(r(z_1)) - H_0} (\mathsf{S} \otimes \mathsf{E}) \frac{1}{z_2 - K_V(r(z_2)) - H_0} \right]. \tag{B.77}$$

This equation contains only terms linear in $r(z_1, z_2)$, so this can be solved algebraically,

$$r(z_1, z_2) = \frac{z_2 - z_1 + K_V(r(z_1)) + K_V(r(z_2))}{z_2 - z_1} \tag{B.78}$$

$$\times \tau \left[\frac{1}{z_1 - K_V(r(z_1)) - H_0} (\mathsf{S} \otimes \mathsf{E}) \frac{1}{z_2 - K_V(r(z_2)) - H_0} \right]. \tag{B.79}$$

The resulting expression for $r(z_1, z_2)$ can be inserted in equation (B.72).

$$\mathbf{r}_{ij}(z_1, z_2) = \tau \left[(E_{ji} \otimes \mathbb{1}_{\mathcal{E}}) \frac{1}{z_1 - K_V(r(z_1)) - H_0} \frac{1}{z_2 - K_V(r(z_2)) - H_0} \right] \tag{B.80}$$

$$\times \frac{K_V\left(r(z_1)\right) - K_V\left(r(z_2)\right)}{r(z_1) - r(z_2)} \times \frac{z_2 - z_1 + K_V(r(z_1)) + K_V(r(z_2))}{z_2 - z_1} \tag{B.81}$$

$$\times \tau \left[\frac{1}{z_1 - K_V(r(z_1)) - H_0} (\mathsf{S} \otimes \mathsf{E}) \frac{1}{z_2 - K_V(r(z_2)) - H_0} \right] \tag{B.82}$$

$$+ \tau \left[(E_{ji} \otimes \mathbb{1}_{\mathcal{E}}) \frac{1}{z_1 - K_V(r(z_1)) - H_0} (\mathsf{S} \otimes \mathsf{E}) \frac{1}{z_2 - K_V(r(z_2)) - H_0} \right]. \tag{B.83}$$

All that is left to do now, is to expand one of the remaining two-point functions,

$$\tau \left[(E_{ji} \otimes \mathbb{1}_{\mathcal{E}}) \frac{1}{z_1 - K_V(r(z_1)) - H_0} \frac{1}{z_2 - K_V(r(z_2)) - H_0} \right] \tag{B.84}$$

$$= \frac{\mathbf{r}_{ij}(z_1) - \mathbf{r}_{ij}(z_2)}{z_2 - z_1 - K_V(r(z_2)) + K_V(r(z_1))}. \tag{B.85}$$

This can be inserted into the general equation for $\mathbf{r}(z_1, z_2)$,

$$\mathbf{r}_{ij}(z_1, z_2) = \frac{\mathbf{r}_{ij}(z_1) - \mathbf{r}_{ij}(z_2)}{z_2 - z_1} \times \frac{K_V\left(r(z_1)\right) - K_V\left(r(z_2)\right)}{r(z_1) - r(z_2)} \tag{B.86}$$

$$\times \tau \left[\frac{1}{z_1 - K_V(r(z_1)) - H_0} (\mathsf{S} \otimes \mathsf{E}) \frac{1}{z_2 - K_V(r(z_2)) - H_0} \right] \tag{B.87}$$

$$+ \tau \left[(E_{ji} \otimes \mathbb{1}_{\mathcal{E}}) \frac{1}{z_1 - K_V(r(z_1)) - H_0} (\mathsf{S} \otimes \mathsf{E}) \frac{1}{z_2 - K_V(r(z_2)) - H_0} \right]. \tag{B.88}$$

If we clean up our notation a bit, this gives us the required result,

$$\mathbf{r}(z_1, z_2) = \frac{\mathbf{r}(z_1) - \mathbf{r}(z_2)}{z_2 - z_1} \times \frac{K_V\left(r(z_1)\right) - K_V\left(r(z_2)\right)}{r(z_1) - r(z_2)} \tag{B.89}$$

$$\times \operatorname{Tr} \mathbb{E}\left[\frac{1}{z_1 - K_V(r(z_1)) - H_0}(\sigma(0) \otimes \mathsf{E})\frac{1}{z_2 - K_V(r(z_2)) - H_0}\right] \tag{B.90}$$

$$+ \mathbb{E}\left[\frac{1}{z_1 - K_V(r(z_1)) - H_0}(\sigma(0) \otimes \mathsf{E})\frac{1}{z_2 - K_V(r(z_2)) - H_0}\right]. \tag{B.91}$$

The validity of this calculation can be expended to $\mathbb{C}\backslash\mathbb{R}$ by a repeat of the arguments given in section 4.3 to argue the extension of theorem 4.2 to theorem 4.6.

□

B.3 Proof of lemma 4.19

Proof. Using holomorphic functional calculus, we can rewrite $\sigma(t)$ in terms of the resolvent of the Hamiltonian as

$$\sigma(t) = \oint_{\Gamma} dz_1 dz_2\, e^{it(z_1 - z_2)}\, \mathbb{E}\left[\frac{1}{z_1 - H}\,(\sigma(0) \otimes \mathsf{E})\,\frac{1}{z_2 - H}\right], \tag{B.92}$$

where Γ is some suitably chosen set of Jordan curves encircling the spectrum of H. In light of the calculations below, care should be taken that the contour used for the integral over z_1 is completely enclosed by te contour use for the integral over z_2.

A similar technique as was used in section 4.5 to calculate the reduced resolvent mapping of H can then be used to calculate explicitly the two-point function $\mathbf{R}(z_1, z_2)$,

$$\mathbf{R}(z_1, z_2) := \mathbb{E}\left[\frac{1}{z_1 - H}\,(\sigma(0) \otimes \mathsf{E})\,\frac{1}{z_2 - H}\right]. \tag{B.93}$$

As in the case of the Hamiltonian specter, it is convenient to introduce a specific notation for the trace of $\mathbf{R}(z_1, z_2)$

$$R(z_1, z_2) = \operatorname{Tr} \mathbb{E}\left[\frac{1}{z_1 - H}\,(\sigma(0) \otimes \mathsf{E})\,\frac{1}{z_2 - H}\right]. \tag{B.94}$$

This expression can be reformulated in terms of the non-interacting Hamiltonian H_0 and the interaction term V,

$$\mathbf{R}(z_1, z_2) = \mathbb{E}\left[\frac{1}{z_1 - H_0 - V}(\sigma(0) \otimes \mathsf{E})\frac{1}{z_2 - H_0 - V}\right]. \tag{B.95}$$

for sufficiently large $|z_1|$ and $|z_2|$, we can expand the resolvents in this expression as convergent Neumann series,

$$\mathbf{R}(z_1, z_2) = \sum_{n_1,n_2}^{\infty} \mathbb{E}\Big[(z_1 - H_0)^{-1} \left(V(z_1 - H_0)^{-1}\right)^{n_1} (\sigma(0) \otimes \mathsf{E}) \tag{B.96}$$

$$\times (z_2 - H_0)^{-1} \left(V(z_2 - H_0))^{-1}\right)^{n_2} \Big] \tag{B.97}$$

To conserve some real estate, we write $A_i = (z_i - H_0)^{-1}$ and $\sigma(0) \otimes \mathsf{E} = M$,

$$\mathbf{R}(z_1, z_2) = \sum_{n_1,n_2}^{\infty} \mathbb{E}\left[A_1 (VA_1)^{n_1} M A_2 (VA_2)^{n_2}\right]. \tag{B.98}$$

As in section 4.4, we rewrite this expression somewhat so that we always have at least one V at our disposal in the summation.

$$\mathbf{R}(z_1, z_2) = \sum_{n_2=0}^{\infty} \mathbb{E}\left[A_1 M (VA)^{n_2}\right] + \sum_{n_1=1}^{\infty} \mathbb{E}\left[A_1 (VA)^{n_1} M A_2 (VA)^{n_2}\right]. \tag{B.99}$$

The first term in this equation can be recombined into a fractional form,

$$\sum_{n_2=0}^{\infty} \mathbb{E}\left[A_1 M (VA_2)^{n_2}\right] = \mathbb{E}\left[AM \frac{1}{A_2^{-1} - V}\right]. \tag{B.100}$$

For the moment, we put this term to the side and concentrate on the remaining summation,

$$\sum_{n_1=1,n_2=0}^{\infty} \mathbb{E}\left[A_1 (VA)^{n_1} M A_2 (VA)^{n_2}\right]. \tag{B.101}$$

This can be rewritten in terms of free cumulants as,

$$\sum_{n_1=0,n_2=0}^{\infty} \sum_{\pi \in NC} k_\pi\Big(A_1, \dot{V}, A_1, \underbrace{V, A_1, \ldots, V, A_1}_{n_1 \text{ times}}, M, A_2, \underbrace{V, A_2, \ldots, V, A_2}_{n_2 \text{ times}}\Big) \tag{B.102}$$

We can rearrange the terms in the sum over NC according to the number of elements connected by the bridge that starts at the dotted V, the first V which appears in the above expansion. Since A_i and V as well as M and V form free couples, the only non-zero cumulants are those which correspond to partitions where the bridges connect only A's and M or only V's. For any n_1, n_2, there are exactly $(n_1 + n_2 + 1)$ V's, so that the bridge that contians $\dot{V}$ connects at most $(n_1 + n_2 + 1)$ elements and at least one; $\dot{V}$.

As in the plain free case, we collect the indices of the V's connected to $\dot{V}$ which occur *before* M in the set X and all indices of V's connected to $\dot{V}$ which occur

after M in the set Y.

$$\sum_{n_1,n_2=0}^{\infty}\sum_{s=1}^{n_1}\sum_{t=0}^{n_2}\sum_{\substack{X,\\ |X|=s,\,2\in X\\ X\subset[3,2n_1-1]}}\sum_{\substack{Y,|Y|=t,\\ Y\subset[2n_1+3,2(n_1+n_2)+1]}}\sum_{\pi\in NC} \tag{B.103}$$

$$k_\pi\Big(A_1,\dot{V},A_1,\underbrace{V,A_1,\ldots,V,A_1}_{n_1\text{ times}},M,A_2,\underbrace{V,A_2,\ldots,V,A_2}_{n_2\text{ times}}\Big) \tag{B.104}$$

If $X=\{x_1,\ldots,x_s\}$, $Y=\{y_1,\ldots,y_t\}$ and $y_{t+1}:=2(n_1+n_2)+4$, then π can be further decomposed as

$$\pi=(X\hat{\cup}Y)\cup\sigma_1\cup\cdots\sigma_{(s-1)}\cup\mu\cup\gamma_1\cup\cdots\gamma_t, \tag{B.105}$$

such that σ_k $(k<s)$ is a non-crossing partition of $\{x_k+1,x_k+2,\ldots,x_{k+1}-1\}$, μ is a non-crossing partition of $\{x_s+1,x_s+2,\ldots,y_1-1\}$ and γ_k $(k\leq t)$ is a non-crossing partition of $\{y_k+1,y_k+2,\ldots,y_{k+1}-1\}$. We gave the $\cup$ in $X\hat{\cup}Y$ a hat, to signify that its meaning is different from the other $\cup$ signs. $X\hat{\cup}Y$ is a union of index-sets, which indicate to which V's, $\dot{V}$ is connected. The other $\cup$ signs indicate the disjoint union of partitions of subsets to form a partition of the disjoint union of the subsets.

We make a distinction between the partitions σ_k, γ_k and μ based on their arguments. Any σ_k has as arguments a series of the form,

$$A_1,V,A_1,\ldots,V,A_1, \tag{B.106}$$

any γ_k $(k<t)$ has as arguments a series of the form,

$$A_2,V,A_2,\ldots,V,A_2 \tag{B.107}$$

γ_t has an argument of the form

$$A_1X,A_2,V,A_2,\ldots,V,A_2, \tag{B.108}$$

where X is some element of the algebra $\mathcal{S}$ and μ has as arguments a series of the form

$$A_1,V,A_1,\ldots,V,A_1,M,A_2,V,A_2,\ldots,V,A_2 \tag{B.109}$$

or

$$A_1X,A_1,V,A_1,\ldots,V,A_1,M,A_2,V,A_2,\ldots,V,A_2 \tag{B.110}$$

if $t = 0$. With this information, equation (B.103) can be rewritten as,

$$\sum_{\substack{n_1=1,\\ n_2=0}}^{\infty} \sum_{s=1}^{n_1} \sum_{\substack{X,\\ |X|=s, 1\in X,\\ X\subset[1,2n_1-1]}} \sum_{\substack{\pi\in NC(2n_1+2n_2+3)\\ \pi=\{X,\dots\}}} \tag{B.111}$$

$$k_\mu\Big(A_1 k_s\left(\dot{\hat{V}}, k_{\sigma_1}(A_1,V,A_1,\dots,V,A_1)\hat{V},\dots,k_{\sigma_{s-1}}(A_1,V,A_1,\dots,V,A_1)\hat{V}\right), \tag{B.112}$$

$$A_1,V,A_1,\dots,V,A_1,M,A_2,V,A_2,\dots,V,A_2\Big) \tag{B.113}$$

$$+\sum_{\substack{n_1=1,\\ n_2=0}}^{\infty} \sum_{s=1}^{n_1}\sum_{t=1}^{n_2} \sum_{\substack{X,\\ |X|=s, 1\in X,\\ X\subset[1,2n_1-1]}} \sum_{\substack{Y,\\ |Y|=t,\\ Y\subset[2n_1+3,2(n_1+n_2)+1]}} \sum_{\substack{\pi\in NC(2n_1+2n_2+3)\\ \pi=\{X\hat{\cup}Y,\dots\}}} \tag{B.114}$$

$$k_{\gamma_t}\Big[A_1 k_s\Big(\dot{\hat{V}}, k_{\sigma_1}(A_1,V,A_1,\dots,V,A_1)\hat{V},\dots,k_{\sigma_{s-1}}(A_1,V,A_1,\dots,V,A_1)\hat{V}, \tag{B.115}$$

$$k_\mu\hat{V}, k_{\gamma_1}\hat{V},\dots,k_{\gamma_{(t-1)}}\hat{V}\Big), A_2,V,A_2,\dots,V,A_2\Big] \tag{B.116}$$

which we abbreviate to,

$$\sum_{\substack{n_1=1,\\ n_2=0}}^{\infty} \sum_{s=1}^{n_1} \sum_{\substack{X,\\ |X|=s, 1\in X,\\ X\subset[1,2n_1-1]}} \sum_{\substack{\pi\in NC(2n_1+2n_2+3)\\ \pi=\{X,\dots\}}} \tag{B.117}$$

$$k_\mu\Big(A_1 k_s\left(\dot{\hat{V}}, k_{\sigma_1}\hat{V},\dots,k_{\sigma_{s-1}}\hat{V}\right), A_1,V,A_1,\dots,V,A_1,M,A_2,V,A_2,\dots,V,A_2\Big) \tag{B.118}$$

$$+\sum_{\substack{n_1=1,\\ n_2=0}}^{\infty} \sum_{s=1}^{n_1}\sum_{t=1}^{n_2} \sum_{\substack{X,\\ |X|=s, 1\in X,\\ X\subset[1,2n_1-1]}} \sum_{\substack{Y,\\ |Y|=t,\\ Y\subset[2n_1+3,2(n_1+n_2)+1]}} \sum_{\substack{\pi\in NC(2n_1+2n_2+3)\\ \pi=\{X\hat{\cup}Y,\dots\}}} \tag{B.119}$$

$$k_{\gamma_t}\Big[A_1 k_{s+t}\Big(\dot{\hat{V}}, k_{\sigma_1}\hat{V},\dots,k_{\sigma_{s-1}}\hat{V}, k_\mu\hat{V}, k_{\gamma_1}\hat{V},\dots,k_{\gamma_{(t-1)}}\hat{V}\Big), A_2,V,A_2,\dots,V,A_2\Big] \tag{B.120}$$

With the usual re-summations, this amount to,

$$\mathbb{E}\left[A_1 K_V(\mathbf{R}(z_1))\frac{1}{z_1-H}(\sigma(0)\otimes \mathsf{E})\frac{1}{z_2-H}\right] \tag{B.121}$$

$$+\sum_{s,t}\mathbb{E}\left[A_1 k_{s+t}\left(V,\mathbf{R}(z_1)V,\dots,\mathbf{R}(z_1)V,\mathbf{R}(z_1,z_2)V,\mathbf{R}(z_2)V,\dots,\mathbf{R}(z_2)V\right)\frac{1}{z_2-H}\right] \tag{B.122}$$

If we denote

$$\mathbf{L} = \sum_{s,t} k_{s+t}\left(V, \mathbf{R}(z_1)V, \ldots, \mathbf{R}(z_1)V, \mathbf{R}(z_1, z_2)V, \mathbf{R}(z_2)V, \ldots, \mathbf{R}(z_2)V\right) \tag{B.123}$$

and

$$\mathbf{K} = K_V(\mathbf{R}(z_1)) \tag{B.124}$$

and collect the term (B.100) from storage, the total amounts to

$$\mathbb{E}\left[A_1 M \frac{1}{A_2^{-1} - V}\right] + \mathbb{E}\left[A_1 \mathbf{L} \frac{1}{A_2^{-1} - V}\right] + \mathbb{E}\left[A_1 \mathbf{K} \frac{1}{A_1^{-1} - V} M \frac{1}{A_2^{-1} - V}\right]. \tag{B.125}$$

As in the proof of lemma 4.13, we can use this equation as a starting point to reiterate the above calculation. This results in,

$$\sum_{n=0}^{\infty} \mathbb{E}\left[A_1 (\mathbf{K} A_1)^n M \frac{1}{A_2^{-1} - V}\right] + \mathbb{E}\left[A_1 (\mathbf{K} A_1)^n \mathbf{L} \frac{1}{A_2^{-1} - V}\right]. \tag{B.126}$$

After symmetrizing and summing up as Neumann series, this leads us to a self-consistent equation for $\mathbf{R}(z_1, z_2)$,

$$\begin{aligned} \mathbf{R}(z_1, z_2) =& \mathbb{E}\left[\frac{1}{z_1 - K_V(\mathbf{R}(z_1)) - H_0} (\sigma(0) \otimes \mathsf{E}) \frac{1}{z_2 - K_V(\mathbf{R}(z_2)) - H_0}\right] && \text{(B.127)} \\ &+ \mathbb{E}\left[\frac{1}{z_1 - K_V(\mathbf{R}(z_1)) - H_0} \mathbf{L}(\mathbf{R}(z_1, z_2)) \frac{1}{z_2 - K_V(\mathbf{R}(z_2)) - H_0}\right]. && \text{(B.128)} \end{aligned}$$

□

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List of publications

Published articles

1. B. Dierckx and A. Verbeure, *Goldstone bosons in Josephson Junctions*, J. Phys. A: Math. Gen. 39 11339-11347 (2006)

2. B. Dierckx, M. Fannes and M. Pogorzelska, *Fermionic quasi-free states and maps in information theory*, Journal of Mathematical Physics 49 032109 (2008)

3. B. Dierckx, M. Fannes and C. Vandenplas, *Additivity of the Renyi entropy of order 2 for positive-partial-transpose-inducing channels*, Phys. Rev. A 77, 060302 (2008)

Articles in preparation

4. B. Dierckx and M. Fannes, *Random interactions between quantum systems*, in preparation

5. B. Dierckx and M. Fannes, *A modified moment-cumulant relation for sums of free random variables*, in preparation

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